

# ELECTRONIC SUPPLEMENTARY INFORMATION

## Revitalizing the concept of bond order through delocalization measure in real space

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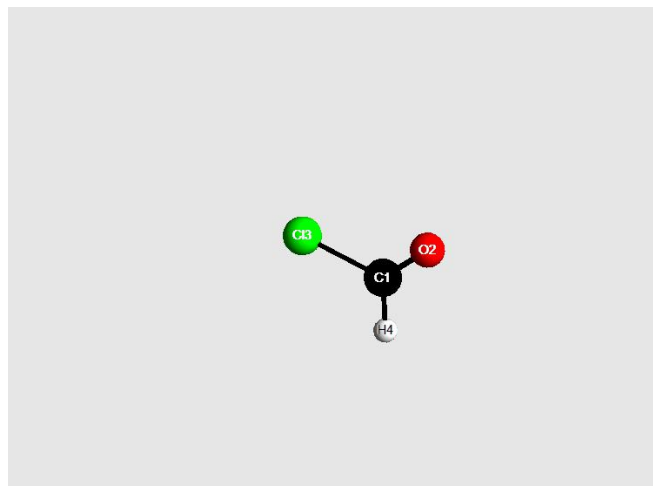
## COMPUTATIONAL DETAILS

All the following molecules have been optimized using the software **GAUSSIAN 09**, and the basis set *6-311++G(2d,2p)*. The delocalization indices have been computed using the software **AIMAll**. It is important to regard that this software uses Müller's approximation for correlated wavefunctions, which in certain cases can differ from the exact result.

The graphs have been plotted to be as congruent as possible with the results. In this way, the atoms have been plotted according to their Cartesian coordinates, and the bonds have been drawn where, and only where, a bond critical point appears. This means that some *non-classical* bonds (mainly hydrogen bonds) appear, and also some classical bonds are not present (particularly in the alkynes, where instead of BCPs, NNACPs are found).

## ACIDS AND DERIVATIVES

### FORMYL CHLORIDE

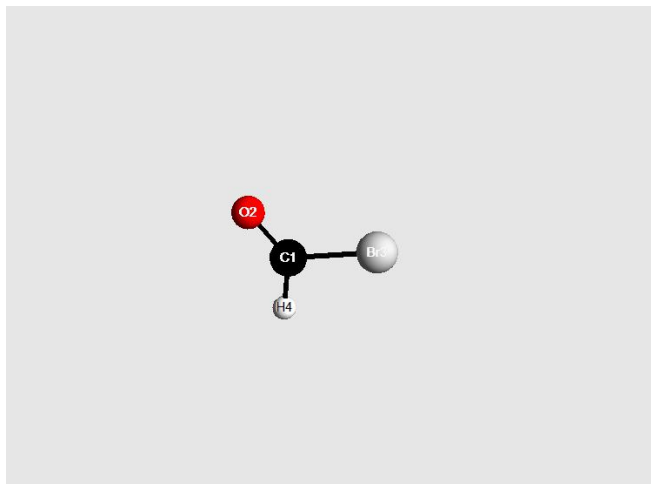


#### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.3330253657
C1	Cl3	0.97807406875
O2	Cl3	0.24647441514
C1	H4	0.87045819503
O2	H4	0.097166897984
Cl3	H4	0.08592645799



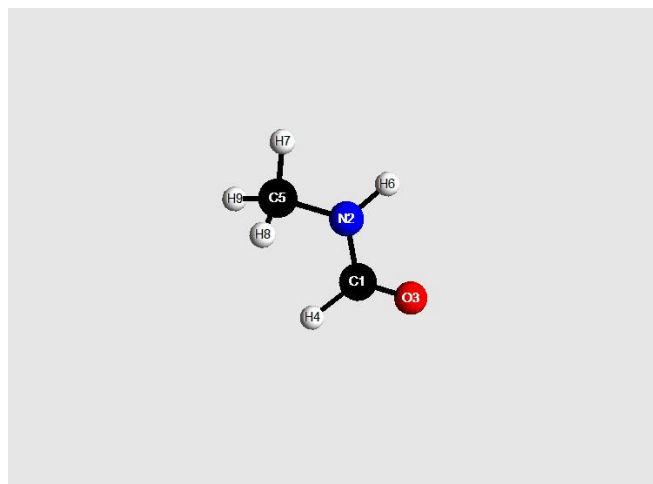
## FORMYL BROMIDE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.3661149919
C1	Br3	1.0016365312
O2	Br3	0.23992451296
C1	H4	0.86977618765
O2	H4	0.095251082632
Br3	H4	0.089780608627

## METHYL FORMAMIDE



### HARTREE-FOCK

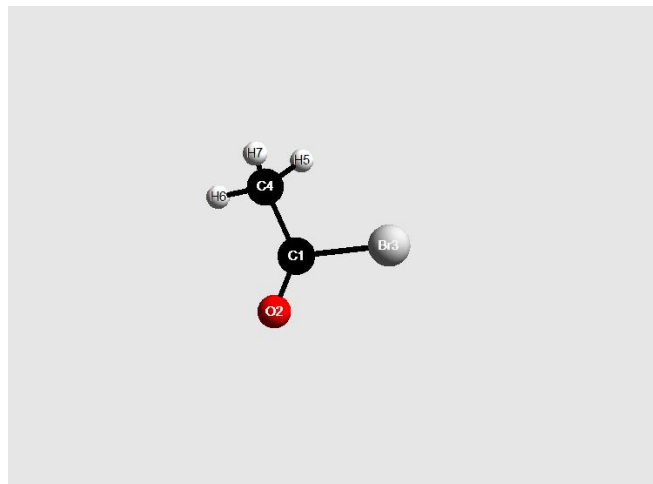
Atom A	Atom B	Delocalization index
C1	N2	0.89987749577
C1	O3	1.1271647675
N2	O3	0.27608560649
C1	H4	0.85933802616
N2	H4	0.07981833403
O3	H4	0.11391747209
C1	C5	0.020528479494
N2	C5	0.89947302224
O3	C5	0.014598677515
H4	C5	0.009980549067
C1	H6	0.015038819222
N2	H6	0.79877248319
O3	H6	0.012748411122
H4	H6	0.0091490596173
C5	H6	0.016769894754
C1	H7	0.0053656109483
N2	H7	0.067875649466
O3	H7	0.0019925190519
H4	H7	0.0016590989037
C5	H7	0.94006136212
H6	H7	0.0034951933484
C1	H8	0.004855531977
N2	H8	0.070402779616
O3	H8	0.0041233563498
H4	H8	0.0036551276077
C5	H8	0.93852262705
H6	H8	0.0031326946793
H7	H8	0.039146199001
C1	H9	0.0048579547529
N2	H9	0.070410363019

O3	H9	0.0041232730315
H4	H9	0.0036550990968
C5	H9	0.93853170117
H6	H9	0.003132677093
H7	H9	0.039145975525
H8	H9	0.040682228933

#### CCSD

Atom A	Atom B	Delocalization index
C1	N2	0.893676114
C1	O3	1.1098961686
N2	O3	0.19906342308
C1	H4	0.74954341717
N2	H4	0.058751173405
O3	H4	0.085160110174
C1	C5	0.021203032611
N2	C5	0.82848216253
O3	C5	0.013653062505
H4	C5	0.011278472214
C1	H6	0.015194736212
N2	H6	0.71452198606
O3	H6	0.01469381867
H4	H6	0.0084911425876
C5	H6	0.015709425935
C1	H7	0.0048306945395
N2	H7	0.04910901147
O3	H7	0.001842961334
H4	H7	0.0015344448999
C5	H7	0.81375408618
H6	H7	0.0033974307651
C1	H8	0.0048341029046
N2	H8	0.050938494017
O3	H8	0.0039235075916
H4	H8	0.0040953268073
C5	H8	0.81040116643
H6	H8	0.0028103064721
H7	H8	0.030631481894
C1	H9	0.0048328533595
N2	H9	0.05094653077
O3	H9	0.0039235487635
H4	H9	0.0040955500105
C5	H9	0.81040463661
H6	H9	0.002810332879
H7	H9	0.030631113139
H8	H9	0.031650329919

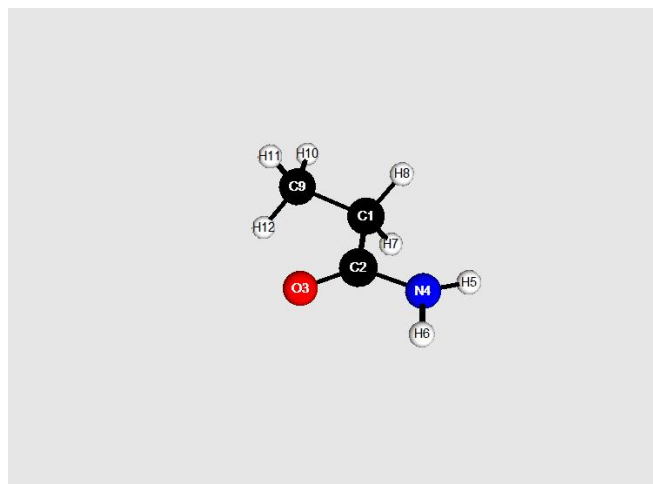
## ACETYL BROMIDE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.3217120271
C1	Br3	0.92972329653
O2	Br3	0.23898233824
C1	C4	0.92976437384
O2	C4	0.10063503422
Br3	C4	0.098447353641
C1	H5	0.049833647722
O2	H5	0.016846385274
Br3	H5	0.018232263041
C4	H5	0.94659318784
C1	H6	0.039606221507
O2	H6	0.016681979976
Br3	H6	0.018400376525
C4	H6	0.951940723
H5	H6	0.033672360478
C1	H7	0.049813861562
O2	H7	0.01684644479
Br3	H7	0.018226545412
C4	H7	0.94652032216
H5	H7	0.035751291339
H6	H7	0.033672962522

## PROPANAMIDE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.89525265736
C1	O3	0.10421502355
C2	O3	1.1066666856
C1	N4	0.086180200616
C2	N4	0.86759094791
O3	N4	0.2685540312
C1	H5	0.0052922484151
C2	H5	0.014080175737
O3	H5	0.015021925846
N4	H5	0.82500642109
C1	H6	0.0075988371636
C2	H6	0.014771674539
O3	H6	0.01205592796
N4	H6	0.80361955086
H5	H6	0.014989103092
C1	H7	0.94647229976
C2	H7	0.045484157452
O3	H7	0.014400009876
N4	H7	0.014368662922
H5	H7	0.0020182528951
H6	H7	0.00036882113479
C1	H8	0.94727633272
C2	H8	0.042309322608
O3	H8	0.014026902856
N4	H8	0.017196429238
H5	H8	0.0020246203236
H6	H8	0.00062328269686
H7	H8	0.041434146053
C1	C9	0.98138700569
C2	C9	0.032169892618

O3	C9	0.034402919058
N4	C9	0.0091401212949
H5	C9	0.00077494000017
H6	C9	0.0013849150176
H7	C9	0.038905822186
H8	C9	0.038645687465
C1	C1	0.045905999909
C2	C1	0.0087017964978
O3	C1	0.0041208464156
N4	C1	0.0016769598461
H5	C1	5.6767880212e-05
H6	C1	0.00034172224763
H7	C1	0.0037442982882
H8	C1	0.003649510415
C9	C1	0.96712670336
C1	H11	0.042648133465
C2	H11	0.0033239714296
O3	H11	0.011973506732
N4	H11	0.00086641311157
H5	H11	0.00010028450021
H6	H11	4.6004393539e-05
H7	H11	0.010919335312
H8	H11	0.0033523157451
C9	H11	0.95895726803
C1	H11	0.041793911485
C1	H12	0.041857366189
C2	H12	0.0029924234043
O3	H12	0.015913353774
N4	H12	0.0008968726709
H5	H12	0.00012051453992
H6	H12	5.0235878737e-05
H7	H12	0.0033934923558
H8	H12	0.010730461182
C9	H12	0.95676165973
C1	H12	0.041254078137
H11	H12	0.040407606445

#### CCSD

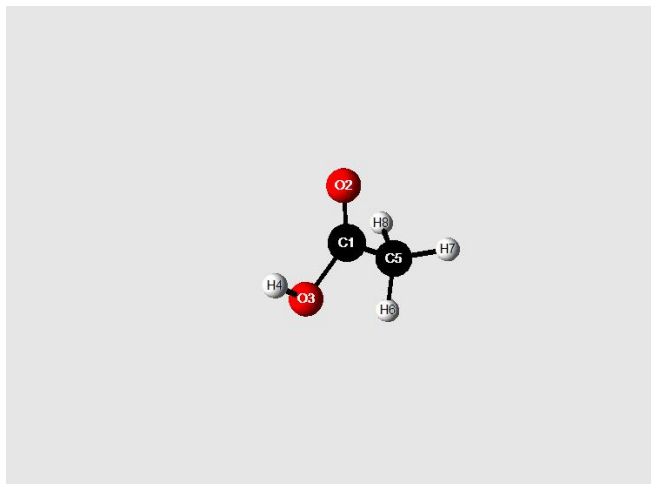
Atom A	Atom B	Delocalization index
C1	C2	0.78069968913
C1	O3	0.079743226616
C2	O3	1.0921866533
C1	N4	0.067376294355
C2	N4	0.86584974915
O3	N4	0.19294136089
C1	H5	0.0060732912137
C2	H5	0.014187026411
O3	H5	0.013987219691

N4	H5	0.738409882
C1	H6	0.0067579231918
C2	H6	0.014928621401
O3	H6	0.013961917972
N4	H6	0.72393600959
H5	H6	0.013836386544
C1	H7	0.81173413481
C2	H7	0.035670017264
O3	H7	0.011563556968
N4	H7	0.011290381509
H5	H7	0.0022441953377
H6	H7	0.00041412596188
C1	H8	0.81252671136
C2	H8	0.031908865905
O3	H8	0.01132972386
N4	H8	0.016084717155
H5	H8	0.0027843123722
H6	H8	0.00067136660556
H7	H8	0.03234662209
C1	C9	0.84426586342
C2	C9	0.027445646396
O3	C9	0.034483625584
N4	C9	0.0069278449296
H5	C9	0.00077103527478
H6	C9	0.0012650676583
H7	C9	0.03176115734
H8	C9	0.03146850187
C1	C1	0.036107676359
C2	C1	0.0068374271838
O3	C1	0.0036121730259
N4	C1	0.0013282990463
H5	C1	7.1799914661e-05
H6	C1	0.00036120015508
H7	C1	0.0033072215635
H8	C1	0.0031223591955
C9	C1	0.83201935609
C1	H11	0.033726695874
C2	H11	0.0035516089319
O3	H11	0.011712700223
N4	H11	0.00082930474818
H5	H11	0.00011953467311
H6	H11	6.587137382e-05
H7	H11	0.0087561362855
H8	H11	0.0029513103695
C9	H11	0.82409541338
C1	H11	0.032477369462
C1	H12	0.032705080695
C2	H12	0.0029787167389

O3	H12	0.018873048825
N4	H12	0.00091027056844
H5	H12	0.00018834548193
H6	H12	8.0777219383e-05
H7	H12	0.0029233951154
H8	H12	0.0085721004841
C9	H12	0.82079322461
C1	H12	0.031793985329
H11	H12	0.031642604242



## ACETIC ACID



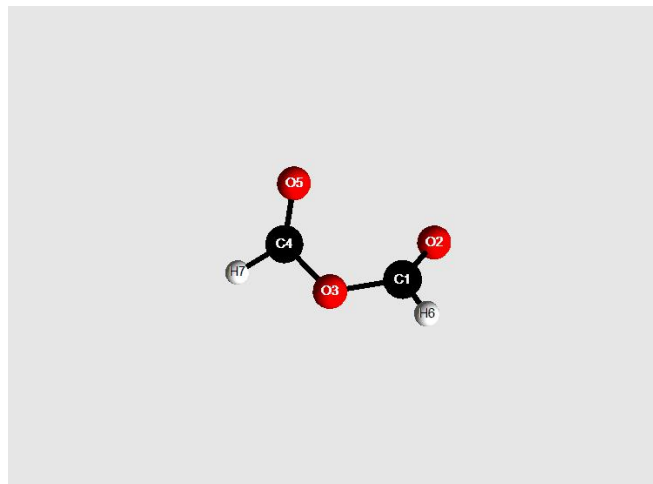
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.0950705796
C1	O3	0.71452440487
O2	O3	0.29967932757
C1	H4	0.008028202658
O2	H4	0.010906392892
O3	H4	0.54625184352
C1	C5	0.90741944738
O2	C5	0.10887855471
O3	C5	0.090019147777
H4	C5	0.0066720075387
C1	H6	0.034275302696
O2	H6	0.013585237433
O3	H6	0.020109545296
H4	H6	0.00055269640774
C5	H6	0.961381206
C1	H7	0.044854428042
O2	H7	0.017316059022
O3	H7	0.0084651822938
H4	H7	0.00066239380379
C5	H7	0.95508130997
H6	H7	0.036502467966
C1	H8	0.044874639169
O2	H8	0.017316426046
O3	H8	0.0084653172151
H4	H8	0.00066239207795
C5	H8	0.95493295786
H6	H8	0.036503156451
H7	H8	0.037605507383

## CCSD

Atom A	Atom B	Delocalization index
C1	O2	1.0892991564
C1	O3	0.72857265615
O2	O3	0.22345110304
C1	H4	0.0093678748142
O2	H4	0.01638569563
O3	H4	0.55244566948
C1	C5	0.79558576662
O2	C5	0.084877837249
O3	C5	0.073682506959
H4	C5	0.0066732954071
C1	H6	0.025801809375
O2	H6	0.0111110834554
O3	H6	0.020274160824
H4	H6	0.00066784893183
C5	H6	0.82594108914
C1	H7	0.034763502929
O2	H7	0.014215836571
O3	H7	0.0067586282324
H4	H7	0.0007646533776
C5	H7	0.82188745972
H6	H7	0.028728822785
C1	H8	0.034775896347
O2	H8	0.014215751993
O3	H8	0.006758600862
H4	H8	0.00076464582305
C5	H8	0.82181717713
H6	H8	0.028728886376
H7	H8	0.029848469791

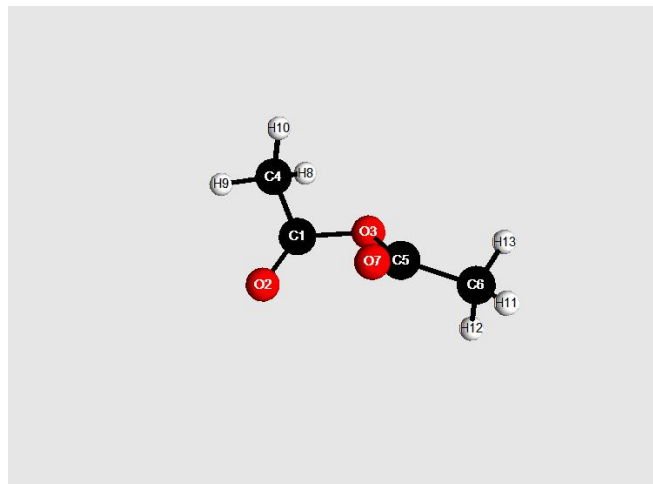
## FORMIC ANHYDRIDE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.2085279016
C1	O3	0.68112506041
O2	O3	0.25502115136
C1	C4	0.011079062377
O2	C4	0.010392174683
O3	C4	0.68057840876
C1	O5	0.010399515258
O2	O5	0.051763474733
O3	O5	0.25506296437
C4	O5	1.2075456977
C1	H6	0.86284069153
O2	H6	0.10342305151
O3	H6	0.077306306976
C4	H6	0.0051665994072
O5	H6	0.0020484824657
C1	H7	0.0051732544537
O2	H7	0.0020493606743
O3	H7	0.077313292514
C4	H7	0.86279948094
O5	H7	0.10342008408
H6	H7	0.00222700343

## ACETIC ANHYDRIDE



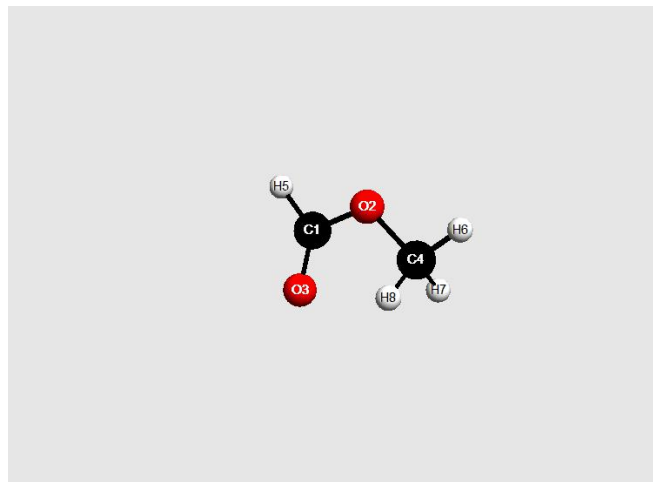
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.1621383999
C1	O3	0.65897039986
O2	O3	0.25247210448
C1	C4	0.91431314549
O2	C4	0.10617877868
O3	C4	0.089233099915
C1	C5	0.010259196454
O2	C5	0.010856572519
O3	C5	0.65862165717
C4	C5	0.0045250232998
C1	C6	0.0045248213545
O2	C6	0.0019623802299
O3	C6	0.089169276881
C4	C6	0.0015264582802
C5	C6	0.91404939063
C1	O7	0.010848152144
O2	O7	0.049642665745
O3	O7	0.25246941356
C4	O7	0.0019656554535
C5	O7	1.1619013813
C6	O7	0.10618365428
C1	H8	0.044422060165
O2	H8	0.016486314938
O3	H8	0.013545335838
C4	H8	0.95452121905
C5	H8	0.00031350011478
C6	H8	5.6337257914e-05
O7	H8	0.00042143436088
C1	H9	0.036564752213
O2	H9	0.016992690341

O3	H9	0.010830798228
C4	H9	0.9579999373
C5	H9	0.00095292068207
C6	H9	0.00036631670038
O7	H9	0.00029869707657
H8	H9	0.035844585846
C1	C1	0.04616349173
O2	C1	0.016945673861
O3	C1	0.01131039224
C4	C1	0.9529094692
C5	C1	0.00024471107293
C6	C1	8.2941733194e-05
O7	C1	0.00067080381086
H8	C1	0.038387961784
H9	C1	0.035839948983
C1	H11	0.00095313903761
O2	H11	0.00029869686984
O3	H11	0.010830716462
C4	H11	0.00036635434406
C5	H11	0.036513429853
C6	H11	0.9580062295
O7	H11	0.016993114883
H8	H11	1.1033370106e-05
H9	H11	9.487138344e-05
C1	H11	1.4304496159e-05
C1	H12	0.00024475934231
O2	H12	0.00067066342371
O3	H12	0.011310645904
C4	H12	8.2995016396e-05
C5	H12	0.046134049652
C6	H12	0.95280518691
O7	H12	0.016945446317
H8	H12	1.043689603e-05
H9	H12	1.4306082183e-05
C1	H12	1.4978137162e-05
H11	H12	0.035839950699
C1	H13	0.00031377098168
O2	H13	0.00042144609883
O3	H13	0.013546099187
C4	H13	5.6422169183e-05
C5	H13	0.044368381787
C6	H13	0.95449182993
O7	H13	0.0164861888
H8	H13	8.9476463862e-06
H9	H13	1.1033819329e-05
C1	H13	1.0438755371e-05
H11	H13	0.035844607181
H12	H13	0.038387829887



## METHYL FORMIATE



## HARTREE-FOCK

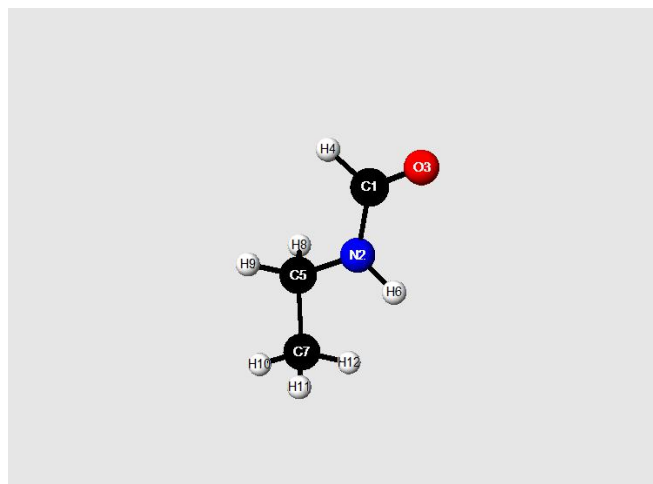
Atom A	Atom B	Delocalization index
C1	O2	0.73955959978
C1	O3	1.1240510304
O2	O3	0.2801039275
C1	C4	0.015308136943
O2	C4	0.76291934299
O3	C4	0.037905894575
C1	H5	0.86001432572
O2	H5	0.08208982446
O3	H5	0.10504926042
C4	H5	0.0089628688714
C1	H6	0.004994332411
O2	H6	0.06931664577
O3	H6	0.0042994021716
C4	H6	0.93621667191
H5	H6	0.001146821169
C1	H7	0.0035455067595
O2	H7	0.070674322958
O3	H7	0.017790626742
C4	H7	0.92787883394
H5	H7	0.00079159388404
H6	H7	0.035349488095
C1	H8	0.0035665684411
O2	H8	0.070694944235
O3	H8	0.017790385465
C4	H8	0.92787273592
H5	H8	0.00079157686206
H6	H8	0.035349248122
H7	H8	0.03580266924

## CCSD

Atom A	Atom B	Delocalization index
C1	O2	0.7543040968
C1	O3	1.1106471773
O2	O3	0.20389950314
C1	C4	0.016928465653
O2	C4	0.72526714779
O3	C4	0.041670422445
C1	H5	0.75127831559
O2	H5	0.063345553384
O3	H5	0.077437074902
C4	H5	0.0083385737069
C1	H6	0.0047974278445
O2	H6	0.052089833087
O3	H6	0.0040426011057
C4	H6	0.80905995982
H5	H6	0.0010989952948
C1	H7	0.0041672864511
O2	H7	0.052170697784
O3	H7	0.019855565634
C4	H7	0.79973686101
H5	H7	0.00086039044157
H6	H7	0.027673761654
C1	H8	0.0041642512649
O2	H8	0.05216614344
O3	H8	0.019854561674
C4	H8	0.79978359081
H5	H8	0.00086035467361
H6	H8	0.027673557141
H7	H8	0.02830604838



## ETHYL FORMAMIDE

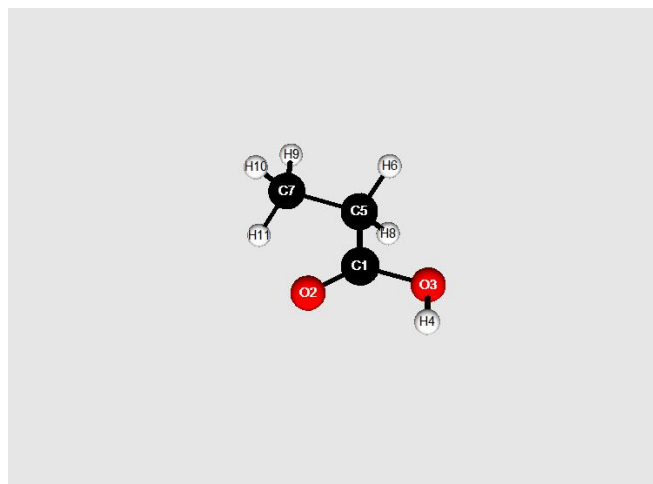


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	N2	0.90095151699
C1	O3	1.1251043041
N2	O3	0.27587481213
C1	H4	0.8595366678
N2	H4	0.079374151498
O3	H4	0.11392421514
C1	C5	0.019475858648
N2	C5	0.87230703505
O3	C5	0.013833622699
H4	C5	0.0095300457424
C1	H6	0.014769678992
N2	H6	0.7964198315
O3	H6	0.012696376218
H4	H6	0.008964005565
C5	H6	0.01653206564
C1	C7	0.0051602553762
N2	C7	0.077255771016
O3	C7	0.0021311067426
H4	C7	0.0016392012262
C5	C7	0.9618338751
H6	C7	0.0076145832863
C1	H8	0.0049239543512
N2	H8	0.070356278075
O3	H8	0.0038650544082
H4	H8	0.0041180983748
C5	H8	0.92596898504
H6	H8	0.0033633134011
C7	H8	0.040092123886
C1	H9	0.0049241760129
N2	H9	0.070344437886

O3	H9	0.0038649334123
H4	H9	0.004118674724
C5	H9	0.92600631609
H6	H9	0.0033636563596
C7	H9	0.040102716269
H8	H9	0.04011779791
C1	C1	0.0010176276324
N2	C1	0.012351291884
O3	C1	0.00067512515704
H4	C1	8.0396674404e-05
C5	C1	0.041939606477
H6	C1	0.00085950175732
C7	C1	0.96452413127
H8	C1	0.003693437467
H9	C1	0.0036934366992
C1	H11	0.00038755156479
N2	H11	0.011570420369
O3	H11	0.00041601924976
H4	H11	0.00025593964609
C5	H11	0.041296235404
H6	H11	0.002348140601
C7	H11	0.96155114319
H8	H11	0.010972305266
H9	H11	0.0037951958259
C1	H11	0.041298914984
C1	H12	0.00038758757723
N2	H12	0.011574147738
O3	H12	0.00041598697431
H4	H12	0.0002559586301
C5	H12	0.041424587132
H6	H12	0.0023482549392
C7	H12	0.9614920843
H8	H12	0.0037952140008
H9	H12	0.010972233954
C1	H12	0.041298858273
H11	H12	0.042192787039

## PROPANOIC ACID

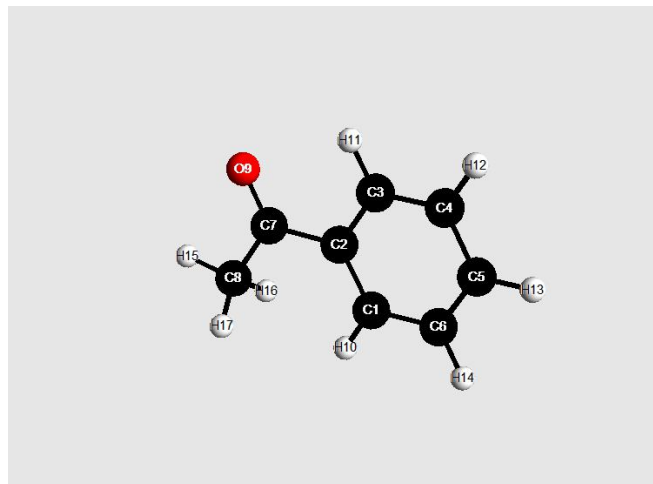


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.0972280704
C1	O3	0.70711268004
O2	O3	0.29621181655
C1	H4	0.0081797773768
O2	H4	0.010827911959
O3	H4	0.54687890879
C1	C5	0.89738950188
O2	C5	0.097462862653
O3	C5	0.090130183975
H4	C5	0.0063100489636
C1	H6	0.046368592719
O2	H6	0.014546462827
O3	H6	0.014999032882
H4	H6	0.00027442189316
C5	H6	0.94121700049
C1	C7	0.034590257665
O2	C7	0.031185127417
O3	C7	0.0097575811863
H4	C7	0.0011231023197
C5	C7	0.98306007583
H6	C7	0.037044020498
C1	H8	0.046319212419
O2	H8	0.014543490318
O3	H8	0.014997513265
H4	H8	0.00027450921186
C5	H8	0.94118664983
H6	H8	0.038872825203
C7	H8	0.037043764188
C1	H9	0.008761368689
O2	H9	0.0037548343578

O3	H9	0.0017050544693
H4	H9	0.00026668524893
C5	H9	0.045346684993
H6	H9	0.0034909678415
C7	H9	0.9667400517
H8	H9	0.0034915318166
C1	C1	0.0032959201659
O2	C1	0.012175688367
O3	C1	0.00089958476828
H4	C1	3.2644041842e-05
C5	C1	0.042575228104
H6	C1	0.0032258920956
C7	C1	0.95906610186
H8	C1	0.010658902248
H9	C1	0.041375609307
C1	H11	0.0032991298962
O2	H11	0.012170003641
O3	H11	0.0008995139354
H4	H11	3.2634337714e-05
C5	H11	0.042592659954
H6	H11	0.010659956108
C7	H11	0.95912197303
H8	H11	0.0032247903397
H9	H11	0.041377410645
C1	H11	0.040723212717

## ACETOPHENONE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3695517434
C1	C3	0.070750159853
C2	C3	1.3384949028
C1	C4	0.094607720813
C2	C4	0.072988760725
C3	C4	1.4064037399
C1	C5	0.076014902669
C2	C5	0.093623500053
C3	C5	0.076000915579
C4	C5	1.371356792
C1	C6	1.3815010287
C2	C6	0.070705260497
C3	C6	0.09638704267
C4	C6	0.072617975216
C5	C6	1.3943184201
C1	C7	0.051441143548
C2	C7	0.95810097405
C3	C7	0.047799125225
C4	C7	0.0077679249331
C5	C7	0.0087036016116
C6	C7	0.0074957913206
C1	C8	0.015182547534
C2	C8	0.046801668449
C3	C8	0.0059261446669
C4	C8	0.001353486768
C5	C8	0.00093692608314
C6	C8	0.0012749110237
C7	C8	0.93204026918
C1	O9	0.024745120523
C2	O9	0.12479669128

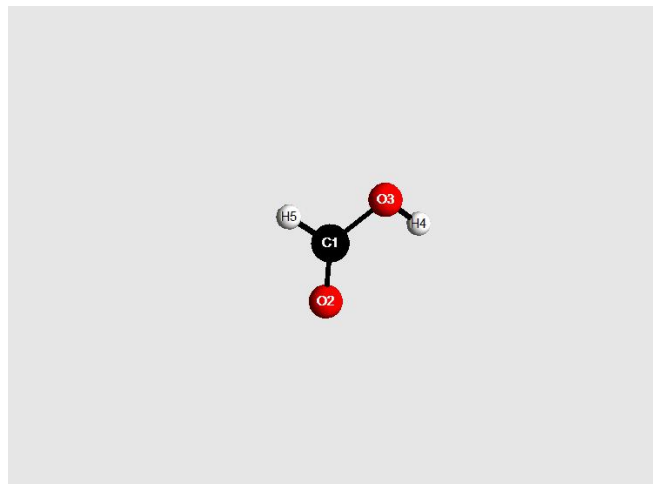
C3	O9	0.046167494704
C4	O9	0.0040280943285
C5	O9	0.010114492012
C6	O9	0.0041238350067
C7	O9	1.2589944622
C8	O9	0.12316355431
C1	C1	0.9617675589
C2	C1	0.045469388117
C3	C1	0.0084314593861
C4	C1	0.0057176984474
C5	C1	0.0080144278787
C6	C1	0.047284383982
C7	C1	0.0054466977702
C8	C1	0.01690770325
O9	C1	0.0014868735667
C1	H11	0.0077669683633
C2	H11	0.041252185532
C3	H11	0.95008295448
C4	H11	0.044475380623
C5	H11	0.0077432201598
C6	H11	0.0050489856088
C7	H11	0.0052038729633
C8	H11	0.00083558066815
O9	H11	0.031585263424
C1	H11	0.0014442025395
C1	H12	0.005766714852
C2	H12	0.0086199696747
C3	H12	0.049642844115
C4	H12	0.97531840182
C5	H12	0.048479207079
C6	H12	0.0084151630262
C7	H12	0.0011154098866
C8	H12	0.00033109736159
O9	H12	0.00019374288587
C1	H12	0.00036678625026
H11	H12	0.0054134800704
C1	H13	0.0085606012258
C2	H13	0.005708435826
C3	H13	0.008371760359
C4	H13	0.047473925756
C5	H13	0.97453586741
C6	H13	0.048697454916
C7	H13	0.00048117800348
C8	H13	8.9016334934e-05
O9	H13	0.0007337173172
C1	H13	0.0012389530321
H11	H13	0.0012074071145
H12	H13	0.0054638542688

C1	H14	0.04938437355
C2	H14	0.0085011010886
C3	H14	0.0060245720186
C4	H14	0.0085384835968
C5	H14	0.049262769512
C6	H14	0.97622018502
C7	H14	0.0010615985885
C8	H14	4.2454888892e-05
O9	H14	0.00057132271709
C1	H14	0.0057422343323
H11	H14	0.00032896991601
H12	H14	0.0013631236397
H13	H14	0.0055780051084
C1	H15	0.0018548332438
C2	H15	0.0073314405706
C3	H15	0.0010720279495
C4	H15	0.00026817704304
C5	H15	0.00011235471299
C6	H15	0.00012937826761
C7	H15	0.035491697831
C8	H15	0.95557607897
O9	H15	0.023512494081
C1	H15	0.0021564046868
H11	H15	8.3401591984e-05
H12	H15	6.3915788435e-05
H13	H15	1.3265318495e-05
H14	H15	1.2460621575e-05
C1	H16	0.0074692464901
C2	H16	0.0049444982027
C3	H16	0.00064152710983
C4	H16	0.0004325897587
C5	H16	0.00049693305441
C6	H16	0.00074524899144
C7	H16	0.044165430694
C8	H16	0.9568050514
O9	H16	0.017935973986
C1	H16	0.0089745140876
H11	H16	9.1926816059e-05
H12	H16	3.1368475109e-05
H13	H16	4.6187997771e-05
H14	H16	2.8897381101e-05
H15	H16	0.037112554665
C1	H17	0.0074804778462
C2	H17	0.0049515524384
C3	H17	0.00064122008668
C4	H17	0.00043255989314
C5	H17	0.00049678965745
C6	H17	0.00074511909004

C7	H17	0.044156507674
C8	H17	0.95695288707
O9	H17	0.017932609652
C1	H17	0.0089485301661
H11	H17	9.2017579796e-05
H12	H17	3.1366175111e-05
H13	H17	4.6173369596e-05
H14	H17	2.8890931912e-05
H15	H17	0.037112661311
H16	H17	0.040793065483



## FORMIC ACID



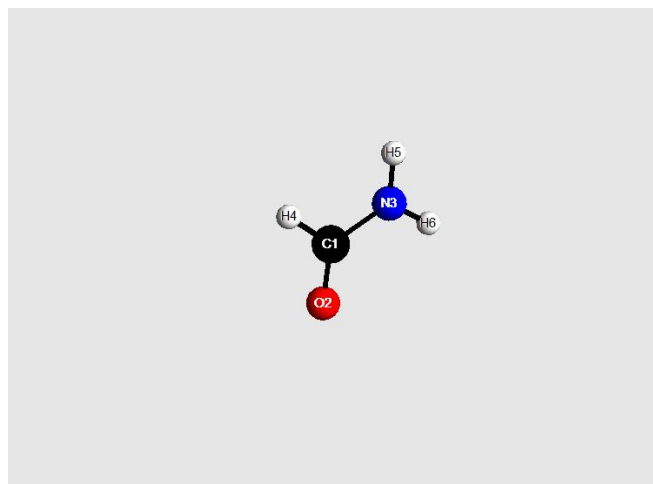
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.1368450354
C1	O3	0.73306972809
O2	O3	0.30261164004
C1	H4	0.0084616455147
O2	H4	0.010100723613
O3	H4	0.54356995525
C1	H5	0.86062857296
O2	H5	0.10467500885
O3	H5	0.081589344706
H4	H5	0.0074425477966

### CCSD

Atom A	Atom B	Delocalization index
C1	O2	1.1247838705
C1	O3	0.74846256593
O2	O3	0.22574926579
C1	H4	0.010048746746
O2	H4	0.015241665017
O3	H4	0.55090974273
C1	H5	0.75160209511
O2	H5	0.077967447808
O3	H5	0.063589817547
H4	H5	0.0077141576969

## FORMAMIDE



### HARTREE-FOCK

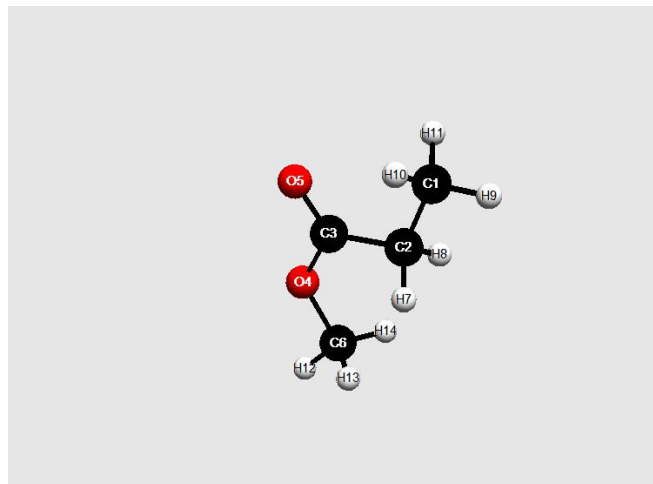
Atom A	Atom B	Delocalization index
C1	O2	1.1330683276
C1	N3	0.8929516223
O2	N3	0.28065351101
C1	H4	0.86456723654
O2	H4	0.1138840505
N3	H4	0.084732024019
C1	H5	0.014317853171
O2	H5	0.014576146589
N3	H5	0.81498560359
H4	H5	0.002298504346
C1	H6	0.014856382046
O2	H6	0.011051724874
N3	H6	0.79503395514
H4	H6	0.0091662358553
H5	H6	0.014899172419

### CCSD

Atom A	Atom B	Delocalization index
C1	O2	1.117896175
C1	N3	0.89042515136
O2	N3	0.204622521
C1	H4	0.7552534709
O2	H4	0.085684786391
N3	H4	0.063744270885
C1	H5	0.014367176307
O2	H5	0.014167836467
N3	H5	0.73256704229
H4	H5	0.0028203338732
C1	H6	0.014856566836
O2	H6	0.012758900852

N3	H6	0.71756693657
H4	H6	0.008485049793
H5	H6	0.013701407513

## METHYL PROPANOATE



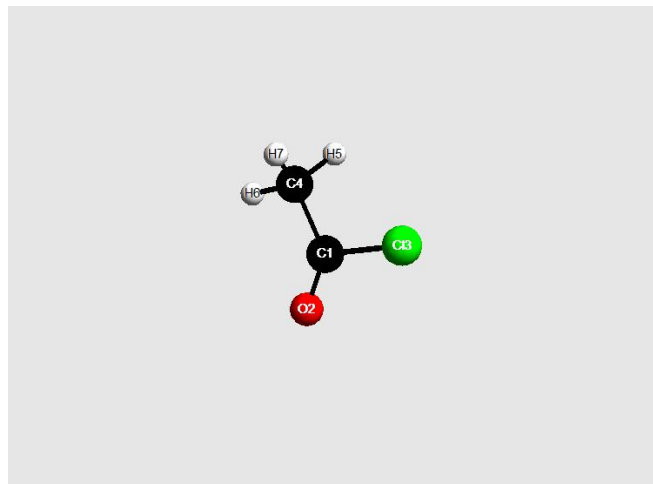
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.97955223845
C1	C3	0.032736957802
C2	C3	0.8938043631
C1	O4	0.0093985215954
C2	O4	0.082470285729
C3	O4	0.70224423235
C1	O5	0.036695924708
C2	O5	0.10511021795
C3	O5	1.1105370389
O4	O5	0.28045617789
C1	C6	0.0019761809807
C2	C6	0.01545439616
C3	C6	0.013502070337
O4	C6	0.77777596096
O5	C6	0.013844852234
C1	H7	0.037295972419
C2	H7	0.93808165585
C3	H7	0.044379369737
O4	H7	0.0082929691636
O5	H7	0.015147343606
C6	H7	0.010236682472
C1	H8	0.037284568844
C2	H8	0.93809736255
C3	H8	0.04433640684
O4	H8	0.0082786842314
O5	H8	0.015144821798
C6	H8	0.010265962345
H7	H8	0.040108165621
C1	H9	0.96676552402
C2	H9	0.045969350447

C3	H9	0.0085541338439
O4	H9	0.0021151206612
O5	H9	0.0043382390556
C6	H9	8.6771438722e-05
H7	H9	0.0036535777573
H8	H9	0.0036706467425
C1	C1	0.95722430609
C2	C1	0.042249230605
C3	C1	0.0032610498247
O4	C1	0.0007108399374
O5	C1	0.014388070542
C6	C1	0.00024701563384
H7	C1	0.0032780802597
H8	C1	0.010370897749
H9	C1	0.041073021145
C1	H11	0.95711375214
C2	H11	0.042248142984
C3	H11	0.0032877527334
O4	H11	0.00071201604903
O5	H11	0.014452290702
C6	H11	0.00024667202182
H7	H11	0.010372627721
H8	H11	0.0032628956081
H9	H11	0.041065504293
C1	H11	0.04000232867
C1	H12	0.00027060971195
C2	H12	0.0022021296495
C3	H12	0.0049893173039
O4	H12	0.070452788261
O5	H12	0.0019675603293
C6	H12	0.92949381013
H7	H12	0.0011647006755
H8	H12	0.0011696131835
H9	H12	2.3234919851e-05
C1	H12	4.5195918416e-05
H11	H12	4.5130961598e-05
C1	H13	0.0010008594345
C2	H13	0.0092058374661
C3	H13	0.0026048936399
O4	H13	0.074306716052
O5	H13	0.0026260512119
C6	H13	0.92609932697
H7	H13	0.014017261713
H8	H13	0.0010596889406
H9	H13	3.4039869732e-05
C1	H13	4.6126707827e-05
H11	H13	0.00031553036717
H12	H13	0.036287459728

C1	H14	0.00099791204156
C2	H14	0.0091982024485
C3	H14	0.0026009589164
O4	H14	0.07430787973
O5	H14	0.0026286711761
C6	H14	0.92615088693
H7	H14	0.0010513885411
H8	H14	0.014022945783
H9	H14	3.3977264077e-05
C1	H14	0.00031552369317
H11	H14	4.5942854633e-05
H12	H14	0.036288836762
H13	H14	0.038950405082

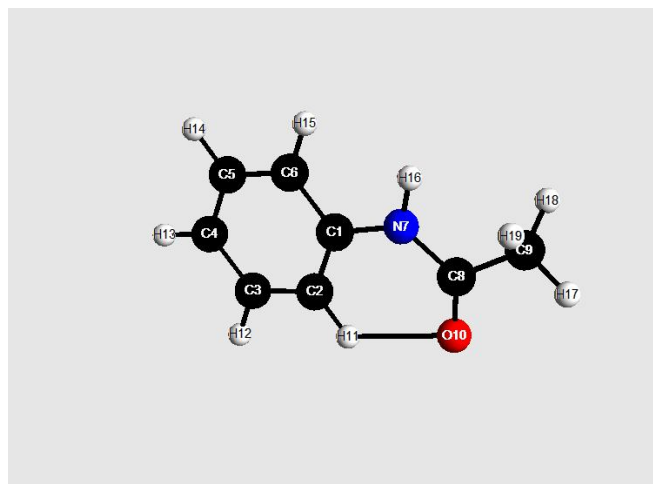
## ACETYL CHLORIDE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	1.2900694627
C1	Cl3	0.91620828457
O2	Cl3	0.24417070836
C1	C4	0.92798430874
O2	C4	0.10210899207
Cl3	C4	0.095613208744
C1	H5	0.048625127176
O2	H5	0.016909069143
Cl3	H5	0.017187850997
C4	H5	0.94807751644
C1	H6	0.039024262691
O2	H6	0.016786446287
Cl3	H6	0.016544376486
C4	H6	0.95344546511
H5	H6	0.034194055202
C1	H7	0.048667693664
O2	H7	0.016928806465
Cl3	H7	0.017125138419
C4	H7	0.94803857708
H5	H7	0.036381688684
H6	H7	0.034200960395

## PHENYL ACETAMIDE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3276502746
C1	C3	0.079205162172
C2	C3	1.3827123058
C1	C4	0.087118327792
C2	C4	0.07085283686
C3	C4	1.3926624079
C1	C5	0.072159933095
C2	C5	0.094710740537
C3	C5	0.077318589977
C4	C5	1.3771240355
C1	C6	1.3101021034
C2	C6	0.063130464193
C3	C6	0.097000635968
C4	C6	0.07310148671
C5	C6	1.4013390684
C1	N7	0.91691017823
C2	N7	0.083908138529
C3	N7	0.011834493308
C4	N7	0.016846163885
C5	N7	0.01266446228
C6	N7	0.10145129686
C1	C8	0.016736888297
C2	C8	0.0065180180709
C3	C8	0.00052847282064
C4	C8	0.0029805012886
C5	C8	0.0012771002049
C6	C8	0.0085902713629
N7	C8	0.86344529335
C1	C9	0.0064552620739
C2	C9	0.001092631413

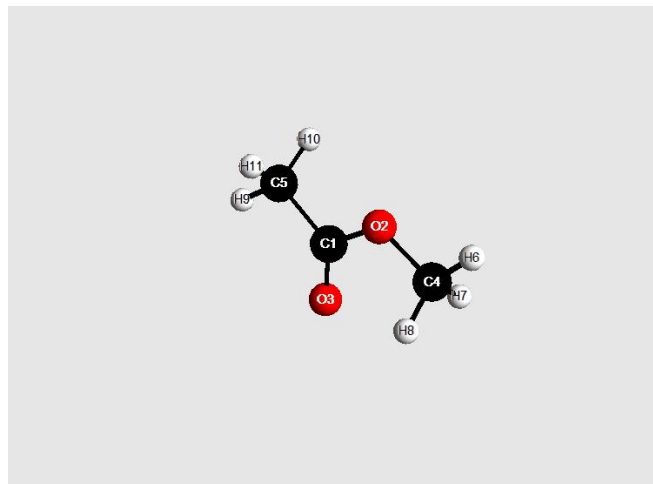


C3	C9	0.00020753575833
C4	C9	0.00035590764799
C5	C9	0.00027280096492
C6	C9	0.0013956358533
N7	C9	0.091017419879
C8	C9	0.90418636704
C1	C1	0.011511089352
C2	C1	0.038435958152
C3	C1	0.0033954867241
C4	C1	0.0034473840822
C5	C1	0.0013050188538
C6	C1	0.004977285596
N7	C1	0.24345342297
C8	C1	1.1163166736
C9	C1	0.113491054
C1	H11	0.043434623673
C2	H11	0.94026704351
C3	H11	0.041397722945
C4	H11	0.0072064967354
C5	H11	0.0048331387014
C6	H11	0.0066956221681
N7	H11	0.0060478171996
C8	H11	0.0011092524635
C9	H11	0.00063007107677
C1	H11	0.050009038044
C1	H12	0.0086109814521
C2	H12	0.049080809275
C3	H12	0.97445213317
C4	H12	0.04887939454
C5	H12	0.0087923630336
C6	H12	0.006075834167
N7	H12	0.001394997793
C8	H12	2.5254093138e-05
C9	H12	1.7882605661e-05
C1	H12	0.00018628742825
H11	H12	0.0055438114131
C1	H13	0.0056876665916
C2	H13	0.008692362597
C3	H13	0.049615911021
C4	H13	0.9790009722
C5	H13	0.049449443134
C6	H13	0.0088162965517
N7	H13	0.0013534243748
C8	H13	0.00019921601736
C9	H13	2.8905524995e-05
C1	H13	0.00034336642735
H11	H13	0.0010682199502
H12	H13	0.0056233655622

C1	H14	0.0085159157595
C2	H14	0.0060970075529
C3	H14	0.0087013189857
C4	H14	0.047744300596
C5	H14	0.97535413824
C6	H14	0.050568863702
N7	H14	0.0014108746691
C8	H14	0.00016447367637
C9	H14	6.3119821758e-05
C1	H14	7.1215199944e-05
H11	H14	0.000305641965
H12	H14	0.0014707280322
H13	H14	0.0055040137739
C1	H15	0.048370302463
C2	H15	0.0073326772446
C3	H15	0.0065194182488
C4	H15	0.0086218261019
C5	H15	0.049748267007
C6	H15	0.97293300611
N7	H15	0.016475668338
C8	H15	0.00055448569114
C9	H15	7.7335177543e-05
C1	H15	0.00063019942124
H11	H15	0.0015535159393
H12	H15	0.00039910409841
H13	H15	0.0013406227417
H14	H15	0.00613857782
C1	H16	0.016043878484
C2	H16	0.0055803137151
C3	H16	0.00093906513046
C4	H16	0.00043164521768
C5	H16	0.0007065647878
C6	H16	0.0082533385133
N7	H16	0.81037433562
C8	H16	0.013861045773
C9	H16	0.0080899895013
C1	H16	0.011607480101
H11	H16	0.00015181767102
H12	H16	0.00023189609977
H13	H16	6.2704510874e-05
H14	H16	5.3369576307e-05
H15	H16	0.0076184971079
C1	H17	0.0013580624926
C2	H17	0.00011765955126
C3	H17	2.9516074561e-05
C4	H17	3.2291013997e-05
C5	H17	5.3359425619e-05
C6	H17	0.00019886655215

N7	H17	0.010008414238
C8	H17	0.0332172294
C9	H17	0.95572799532
C1	H17	0.021247859666
H11	H17	6.2624478279e-05
H12	H17	6.3840499538e-06
H13	H17	2.7054694127e-06
H14	H17	1.3548157492e-05
H15	H17	1.6406277257e-05
H16	H17	0.0011620747759
C1	H18	0.00044946885139
C2	H18	0.00045743425828
C3	H18	5.2746979032e-05
C4	H18	0.00022182882431
C5	H18	4.4212739465e-05
C6	H18	0.00032744900706
N7	H18	0.013733131213
C8	H18	0.041703346555
C9	H18	0.96166121624
C1	H18	0.015220512738
H11	H18	8.5352893575e-05
H12	H18	5.5406014026e-06
H13	H18	1.5481772469e-05
H14	H18	3.5022795074e-06
H15	H18	1.9453512841e-05
H16	H18	0.0025267837622
H17	H18	0.037370574015
C1	H19	0.00044703033832
C2	H19	0.00045922579241
C3	H19	5.2818435142e-05
C4	H19	0.0002242377086
C5	H19	4.4603225984e-05
C6	H19	0.00033054751552
N7	H19	0.013682654415
C8	H19	0.041782177345
C9	H19	0.96161176738
C1	H19	0.015223340151
H11	H19	8.4690143126e-05
H12	H19	5.4316138674e-06
H13	H19	1.5642163704e-05
H14	H19	3.5205057183e-06
H15	H19	1.9315884854e-05
H16	H19	0.0024604048591
H17	H19	0.037366830249
H18	H19	0.041215236875

## METHYL ACETATE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	0.71477920489
C1	O3	1.0929884568
O2	O3	0.27235653662
C1	C4	0.014670590049
O2	C4	0.7635485525
O3	C4	0.039716581533
C1	C5	0.90623457665
O2	C5	0.093472870122
O3	C5	0.10774903002
C4	C5	0.0077697921796
C1	H6	0.005167026357
O2	H6	0.070282817412
O3	H6	0.0045220704037
C4	H6	0.93591785105
C5	H6	0.00099459967863
C1	H7	0.0032622089199
O2	H7	0.071039476333
O3	H7	0.018982956855
C4	H7	0.92708726279
C5	H7	0.00080569172522
H6	H7	0.035820654342
C1	H8	0.0032600846319
O2	H8	0.071040400791
O3	H8	0.018982992627
C4	H8	0.92708781425
C5	H8	0.00080578227702
H6	H8	0.035820468029
H7	H8	0.036200575025
C1	H9	0.035214707419
O2	H9	0.01051147167

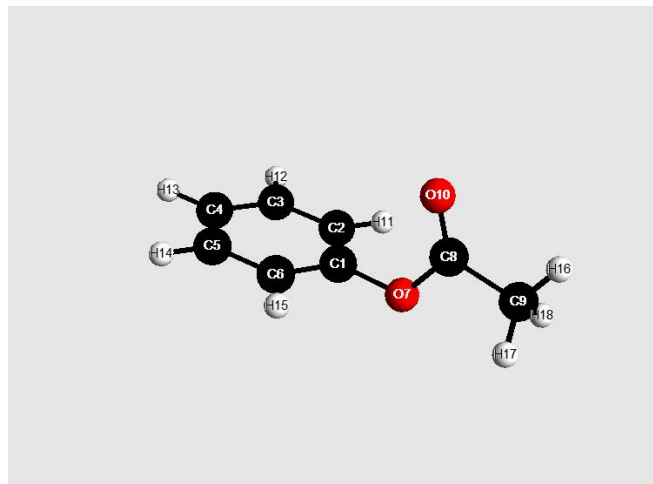
O3	H9	0.018126889022
C4	H9	0.0015498992233
C5	H9	0.95953683385
H6	H9	0.0002563566147
H7	H9	8.8826023098e-05
H8	H9	8.8825418592e-05
C1	C1	0.043298376259
O2	C1	0.013355143727
O3	C1	0.01546994361
C4	C1	0.00042353340934
C5	C1	0.95657214071
H6	C1	4.8216193936e-05
H7	C1	0.00015244609471
H8	C1	0.00025328359624
H9	C1	0.0364392352
C1	H11	0.043339956003
O2	H11	0.013355325264
O3	H11	0.015470046823
C4	H11	0.00042355471705
C5	H11	0.95656412736
H6	H11	4.8216783064e-05
H7	H11	0.00025328700281
H8	H11	0.00015244736358
H9	H11	0.036439135337
C1	H11	0.038874006171

### CCSD

Atom A	Atom B	Delocalization index
C1	O2	0.72848709121
C1	O3	1.0818046631
O2	O3	0.1976756304
C1	C4	0.015763368714
O2	C4	0.72652102258
O3	C4	0.043620014247
C1	C5	0.79501550699
O2	C5	0.076878664833
O3	C5	0.082607379452
C4	C5	0.0071750542067
C1	H6	0.0049207286685
O2	H6	0.052796317134
O3	H6	0.0042119578412
C4	H6	0.80874014666
C5	H6	0.00092518878399
C1	H7	0.0037910895615
O2	H7	0.052459150039
O3	H7	0.021164906434
C4	H7	0.79906530985
C5	H7	0.00083009807245

H6	H7	0.027959487164
C1	H8	0.0037976629574
O2	H8	0.0524542679
O3	H8	0.021164371179
C4	H8	0.79905172143
C5	H8	0.00082990307704
H6	H8	0.027959660293
H7	H8	0.028596209916
C1	H9	0.027957839584
O2	H9	0.0081250482897
O3	H9	0.017164762633
C4	H9	0.0015864799113
C5	H9	0.82511610023
H6	H9	0.00027674365259
H7	H9	0.00010510055296
H8	H9	0.0001050992166
C1	C1	0.032940438097
O2	C1	0.012264191666
O3	C1	0.012055266968
C4	C1	0.00046428491206
C5	C1	0.82260551756
H6	C1	6.1673854498e-05
H7	C1	0.00018606307467
H8	C1	0.00027267071213
H9	C1	0.028656877317
C1	H11	0.032916212532
O2	H11	0.012263818227
O3	H11	0.012055276108
C4	H11	0.0004642919947
C5	H11	0.82261387055
H6	H11	6.1673040308e-05
H7	H11	0.00027266782161
H8	H11	0.00018606025602
H9	H11	0.028656731928
C1	H11	0.030597196716

## PHENYL ACETATE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3293772286
C1	C3	0.075696915059
C2	C3	1.3827368532
C1	C4	0.089902525406
C2	C4	0.072715157997
C3	C4	1.3879026032
C1	C5	0.075704753741
C2	C5	0.097684736291
C3	C5	0.075990273017
C4	C5	1.3878755674
C1	C6	1.3293927
C2	C6	0.064005036814
C3	C6	0.097674914916
C4	C6	0.072713470172
C5	C6	1.3827833191
C1	O7	0.76184289855
C2	O7	0.09834908592
C3	O7	0.011846570858
C4	O7	0.012735384176
C5	O7	0.011848537421
C6	O7	0.098342934571
C1	C8	0.013412202712
C2	C8	0.0054687500362
C3	C8	0.00064681869073
C4	C8	0.001483219329
C5	C8	0.00064663529432
C6	C8	0.0054675062951
O7	C8	0.69732612764
C1	C9	0.006855972493
C2	C9	0.00099233611491

C3	C9	0.00021844151463
C4	C9	0.00015320564238
C5	C9	0.00021849502262
C6	C9	0.00099224057235
O7	C9	0.092075015639
C8	C9	0.90825103306
C1	C1	0.039524828809
C2	C1	0.013776207434
C3	C1	0.0019692178259
C4	C1	0.0019121046423
C5	C1	0.0019698256808
C6	C1	0.013770559616
O7	C1	0.2655544822
C8	C1	1.124464234
C9	C1	0.10671540967
C1	H11	0.047155639332
C2	H11	0.96739865403
C3	H11	0.045758393238
C4	H11	0.0082039915722
C5	H11	0.0058615067227
C6	H11	0.0069443531846
O7	H11	0.014636561924
C8	H11	0.00060774347265
C9	H11	0.00015050854969
C1	H11	0.0019141304681
C1	H12	0.0083940189019
C2	H12	0.049183858818
C3	H12	0.97492085683
C4	H12	0.048329058962
C5	H12	0.0085942373779
C6	H12	0.0059929776648
O7	H12	0.0015286023121
C8	H12	8.5509869597e-05
C9	H12	4.5486322305e-05
C1	H12	0.00013326194124
H11	H12	0.0056439700535
C1	H13	0.0056840112747
C2	H13	0.008589282726
C3	H13	0.049296071125
C4	H13	0.97675707988
C5	H13	0.049292267322
C6	H13	0.0085885044436
O7	H13	0.00096599255718
C8	H13	0.00010094818909
C9	H13	1.1970914714e-05
C1	H13	0.00012726064198
H11	H13	0.0012782531433
H12	H13	0.0055725354354

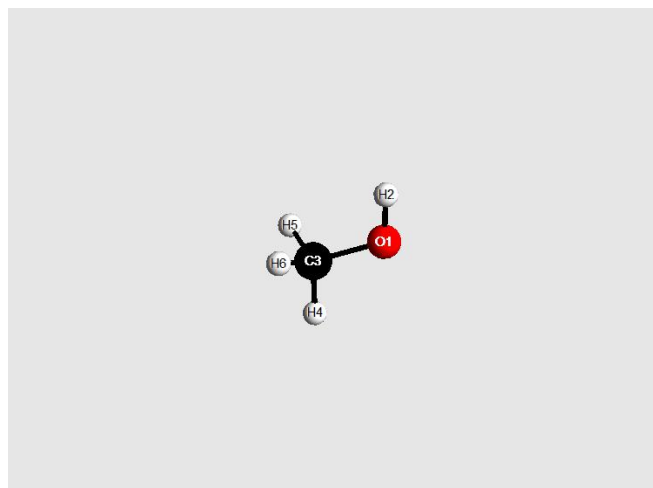


C1	H14	0.0083943441312
C2	H14	0.0059935214576
C3	H14	0.0085936751351
C4	H14	0.048329800814
C5	H14	0.97493688108
C6	H14	0.049194280045
O7	H14	0.0015285655719
C8	H14	8.5491987045e-05
C9	H14	4.5494004902e-05
C1	H14	0.00013326446337
H11	H14	0.00035123721235
H12	H14	0.0014377961346
H13	H14	0.0055722992084
C1	H15	0.04720236245
C2	H15	0.0069444944905
C3	H15	0.0058613758814
C4	H15	0.0082041113435
C5	H15	0.045768717741
C6	H15	0.96738326694
O7	H15	0.014650223499
C8	H15	0.00060680944525
C9	H15	0.00015049055723
C1	H15	0.0019141175095
H11	H15	0.001563824131
H12	H15	0.00035124258113
H13	H15	0.0012782800234
H14	H15	0.0056440616033
C1	H16	0.0013708421388
C2	H16	0.00015969986841
C3	H16	5.0424740226e-05
C4	H16	3.0234904463e-05
C5	H16	5.0425984621e-05
C6	H16	0.00015969060455
O7	H16	0.010512588651
C8	H16	0.035895323426
C9	H16	0.95915614971
C1	H16	0.017855534469
H11	H16	2.2311108584e-05
H12	H16	1.0711563885e-05
H13	H16	2.5690236411e-06
H14	H16	1.0711485088e-05
H15	H16	2.2310834442e-05
C1	H17	0.00039971208213
C2	H17	0.00021093611863
C3	H17	3.4761017191e-05
C4	H17	3.0989513677e-05
C5	H17	2.0811832896e-05
C6	H17	0.00018121543953

O7	H17	0.013326498835
C8	H17	0.044133226851
C9	H17	0.95565041983
C1	H17	0.015822113807
H11	H17	1.2879539814e-05
H12	H17	7.256585267e-06
H13	H17	2.7125260599e-06
H14	H17	4.6871732714e-06
H15	H17	5.9558846911e-05
H16	H17	0.036452574887
C1	H18	0.00039965249027
C2	H18	0.00018134046254
C3	H18	2.0809417572e-05
C4	H18	3.098899929e-05
C5	H18	3.4764174828e-05
C6	H18	0.00021090960919
O7	H18	0.013325753579
C8	H18	0.044114501859
C9	H18	0.95565380386
C1	H18	0.015822156248
H11	H18	5.9557164681e-05
H12	H18	4.6874399351e-06
H13	H18	2.7125770038e-06
H14	H18	7.2567918667e-06
H15	H18	1.288048619e-05
H16	H18	0.036452754826
H17	H18	0.038930906287

# ALCOHOLS

## METHANOL



### HARTREE-FOCK

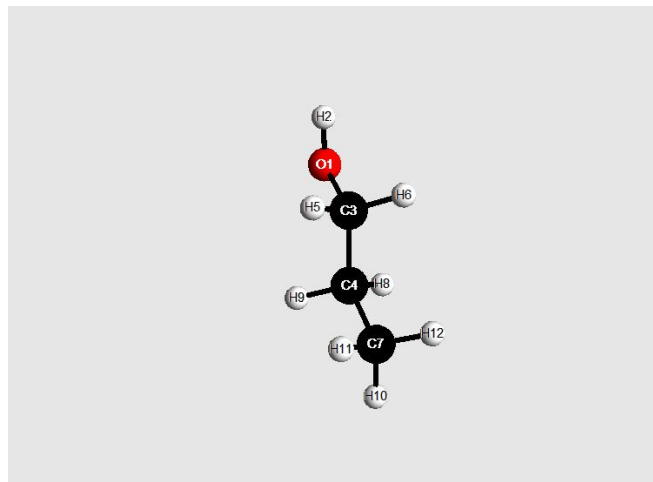
Atom A	Atom B	Delocalization index
O1	H2	0.61756287608
O1	C3	0.82367320207
H2	C3	0.01144520381
O1	H4	0.072767308058
H2	H4	0.0068396357091
C3	H4	0.9314260154
O1	H5	0.082935106253
H2	H5	0.0010829644068
C3	H5	0.93355917232
H4	H5	0.040334829681
O1	H6	0.082934553697
H2	H6	0.0010829844823
C3	H6	0.9335221769
H4	H6	0.040335017722
H5	H6	0.042804466817

### CCSD

Atom A	Atom B	Delocalization index
O1	H2	0.61026420736
O1	C3	0.78500237165
H2	C3	0.013494605823
O1	H4	0.053873076949
H2	H4	0.0063965198233
C3	H4	0.80606603779
O1	H5	0.06176480045
H2	H5	0.0013440351799
C3	H5	0.80762325153
H4	H5	0.031547140534

O1	H6	0.061763742917
H2	H6	0.0013440531951
C3	H6	0.8076434945
H4	H6	0.031547222551
H5	H6	0.033316477661

## PROPANOL

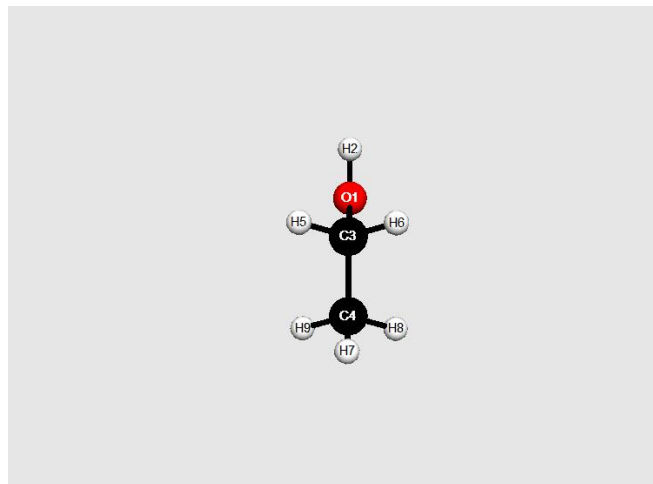


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	H2	0.61798228493
O1	C3	0.7980770785
H2	C3	0.010760908728
O1	C4	0.082700658208
H2	C4	0.0061183974604
C3	C4	0.94016554761
O1	H5	0.082534477226
H2	H5	0.0010165749886
C3	H5	0.91667495667
C4	H5	0.039213134539
O1	H6	0.082535143035
H2	H6	0.0010165925389
C3	H6	0.91667490027
C4	H6	0.039185555947
H5	H6	0.041837242075
O1	C7	0.01177457527
H2	C7	0.0012669267006
C3	C7	0.044968878761
C4	C7	0.98048873183
H5	C7	0.0077003810588
H6	C7	0.007694012291
O1	H8	0.013767161928
H2	H8	0.00032370385043
C3	H8	0.040633753572
C4	H8	0.9468720831
H5	H8	0.010677349053
H6	H8	0.0039532017873
C7	H8	0.041754280492
O1	H9	0.013767172744
H2	H9	0.00032370332729

C3	H9	0.040743968913
C4	H9	0.94685156233
H5	H9	0.0039531987689
H6	H9	0.010677350611
C7	H9	0.041753885957
H8	H9	0.041284518545
O1	O1	0.0020461806173
H2	O1	0.0002701093723
C3	O1	0.0099857020739
C4	O1	0.042178078346
H5	O1	0.00093489485729
H6	O1	0.00093488395936
C7	O1	0.96610200297
H8	O1	0.0037444911067
H9	O1	0.003744534478
O1	H11	0.0014056061803
H2	H11	4.1473567068e-05
C3	H11	0.0066708531096
C4	H11	0.041652498304
H5	H11	0.0066197986997
H6	H11	0.00057271660691
C7	H11	0.96403659272
H8	H11	0.011347377377
H9	H11	0.0035198376208
O1	H11	0.04380940326
O1	H12	0.0014057438024
H2	H12	4.1474972539e-05
C3	H12	0.0066738695342
C4	H12	0.041617773013
H5	H12	0.00057280488299
H6	H12	0.0066199524204
C7	H12	0.96402057133
H8	H12	0.0035198384571
H9	H12	0.011347394572
O1	H12	0.043809600047
H11	H12	0.044481194173

## ETHANOL



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	H2	0.61835846834
O1	C3	0.79978297139
H2	C3	0.01080036898
O1	C4	0.085971316674
H2	C4	0.0063105164843
C3	C4	0.95425229805
O1	H5	0.083001254529
H2	H5	0.0010147877102
C3	H5	0.9204934438
C4	H5	0.041515350638
O1	H6	0.082999674613
H2	H6	0.0010147679089
C3	H6	0.92042913977
C4	H6	0.041507305871
H5	H6	0.041764378408
O1	H7	0.013148942094
H2	H7	0.001490971599
C3	H7	0.043381719004
C4	H7	0.96705531927
H5	H7	0.0037340452406
H6	H7	0.0037340359073
O1	H8	0.012502053014
H2	H8	0.00030170030622
C3	H8	0.040686347127
C4	H8	0.9608981877
H5	H8	0.011158827301
H6	H8	0.0040098882027
H7	H8	0.042118017828
O1	H9	0.012502049766
H2	H9	0.00030170763781

C3	H9	0.040580950092
C4	H9	0.96086095661
H5	H9	0.0040100736147
H6	H9	0.011158807789
H7	H9	0.042118069134
H8	H9	0.041656182426

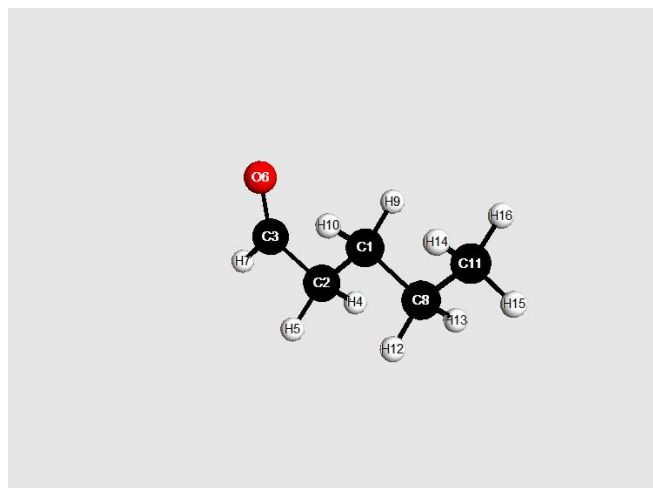
#### CCSD

Atom A	Atom B	Delocalization index
O1	H2	0.61008569398
O1	C3	0.76259235258
H2	C3	0.012705430622
O1	C4	0.070900829844
H2	C4	0.0058779618384
C3	C4	0.82781789474
O1	H5	0.06204730154
H2	H5	0.0013140744611
C3	H5	0.79482089308
C4	H5	0.033783571026
O1	H6	0.062047407931
H2	H6	0.0013141183628
C3	H6	0.794893826
C4	H6	0.033733974993
H5	H6	0.032454031161
O1	H7	0.010479154489
H2	H7	0.0016312247052
C3	H7	0.034737036038
C4	H7	0.83144060907
H5	H7	0.0033236362191
H6	H7	0.0033237518944
O1	H8	0.012652178544
H2	H8	0.0003940691511
C3	H8	0.032354987841
C4	H8	0.82544498758
H5	H8	0.0089851117147
H6	H8	0.0034598187417
H7	H8	0.032501996471
O1	H9	0.012652396847
H2	H9	0.00039408253484
C3	H9	0.032247402982
C4	H9	0.82537251857
H5	H9	0.0034597154942
H6	H9	0.0089851524126
H7	H9	0.032502093626
H8	H9	0.032293960911



# ALDEHYDES AND KETONES

## PENTANAL



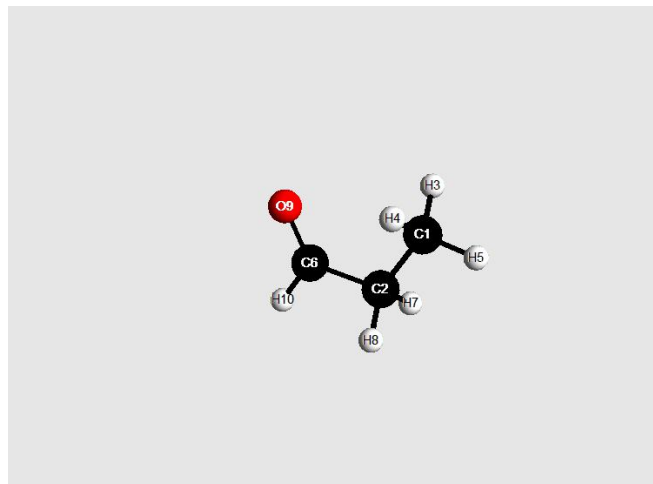
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.96813612277
C1	C3	0.033841651294
C2	C3	0.93888875696
C1	H4	0.036577240318
C2	H4	0.94052639974
C3	H4	0.051913960924
C1	H5	0.036590166913
C2	H5	0.94059811216
C3	H5	0.051897282599
H4	H5	0.042273907069
C1	O6	0.028769782462
C2	O6	0.11208975877
C3	O6	1.3122110767
H4	O6	0.018558793071
H5	O6	0.018554091393
C1	H7	0.0081591508819
C2	H7	0.05003266217
C3	H7	0.88888261522
H4	H7	0.0039075921562
H5	H7	0.0039101010466
O6	H7	0.12564954982
C1	C8	0.96635025697
C2	C8	0.045595774506
C3	C8	0.0079308599596
H4	C8	0.0070812986877
H5	C8	0.0070875488649
O6	C8	0.0035246106981
H7	C8	0.0014302055743

C1	H9	0.94148796921
C2	H9	0.042907249193
C3	H9	0.0036895211686
H4	H9	0.0032620159226
H5	H9	0.010548349589
O6	H9	0.013412343452
H7	H9	0.00047529031447
C8	H9	0.039422040223
C1	C1	0.94153511324
C2	C1	0.042920618145
C3	C1	0.0037097822577
H4	C1	0.010548755708
H5	C1	0.0032645869681
O6	C1	0.013391707499
H7	C1	0.0004748125773
C8	C1	0.039427741743
H9	C1	0.041037127428
C1	C11	0.044400985235
C2	C11	0.0093483701367
C3	C11	0.0015038476825
H4	C11	0.00077326498273
H5	C11	0.0007733777047
O6	C11	0.00023864816952
H7	C11	0.00048107692269
C8	C11	0.9776844149
H9	C11	0.0077087818766
C1	C11	0.0076985755108
C1	H12	0.042546899117
C2	H12	0.0079598262997
C3	H12	0.00064399171584
H4	H12	0.00054949647787
H5	H12	0.0067160346018
O6	H12	0.00067531376992
H7	H12	6.3819745607e-05
C8	H12	0.94861956237
H9	H12	0.010933225463
C1	H12	0.0035394568632
C11	H12	0.043634950768
C1	H13	0.042544538817
C2	H13	0.0079559055561
C3	H13	0.00064487764688
H4	H13	0.0067201333133
H5	H13	0.00054932157588
O6	H13	0.0006750636051
H7	H13	6.3834448654e-05
C8	H13	0.94862589157
H9	H13	0.0035383204148
C1	H13	0.010933937981

C11	H13	0.04366313636
H12	H13	0.044628328693
C1	H14	0.007181382032
C2	H14	0.00077483191828
C3	H14	5.9067988986e-05
H4	H14	0.00034865267933
H5	H14	4.3494028072e-05
O6	H14	4.4635696384e-05
H7	H14	1.7072641269e-05
C8	H14	0.041806171136
H9	H14	0.00053292894978
C1	H14	0.0064016724076
C11	H14	0.96265785783
H12	H14	0.0036874791741
H13	H14	0.011541522009
C1	H15	0.010326458102
C2	H15	0.0019041979637
C3	H15	0.00036177034708
H4	H15	5.001392327e-05
H5	H15	4.9996953464e-05
O6	H15	7.455709697e-05
H7	H15	0.00013474554453
C8	H15	0.042525294342
H9	H15	0.00082937485868
C1	H15	0.00082943970692
C11	H15	0.96661879869
H12	H15	0.0039082420246
H13	H15	0.0039096085717
H14	H15	0.044060114486
C1	H16	0.007178920105
C2	H16	0.00077528585648
C3	H16	5.9069508311e-05
H4	H16	4.3502277515e-05
H5	H16	0.00034860132228
O6	H16	4.4657707011e-05
H7	H16	1.7073439989e-05
C8	H16	0.04181070687
H9	H16	0.0064029168533
C1	H16	0.00053297186433
C11	H16	0.96287130055
H12	H16	0.01154160538
H13	H16	0.0036860870789
H14	H16	0.044460386278
H15	H16	0.044059539085

## PROPANAL



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.98209264359
C1	H3	0.9594262994
C2	H3	0.042833605775
C1	H4	0.95939970405
C2	H4	0.04284637294
H3	H4	0.041286286627
C1	H5	0.96695303923
C2	H5	0.045469486003
H3	H5	0.042055592374
H4	H5	0.042057432242
C1	C6	0.035189576086
C2	C6	0.93773569222
H3	C6	0.0037134916596
H4	C6	0.0037049587414
H5	C6	0.0091392134553
C1	H7	0.038570496132
C2	H7	0.94491772132
H3	H7	0.0032562434857
H4	H7	0.010935520191
H5	H7	0.0036058074265
C6	H7	0.052023599649
C1	H8	0.038591164391
C2	H8	0.94492507885
H3	H8	0.010938027873
H4	H8	0.0032697846443
H5	H8	0.0035956370487
C6	H8	0.052064594939
H7	H8	0.04213510985
C1	O9	0.031120456256
C2	O9	0.11297738119

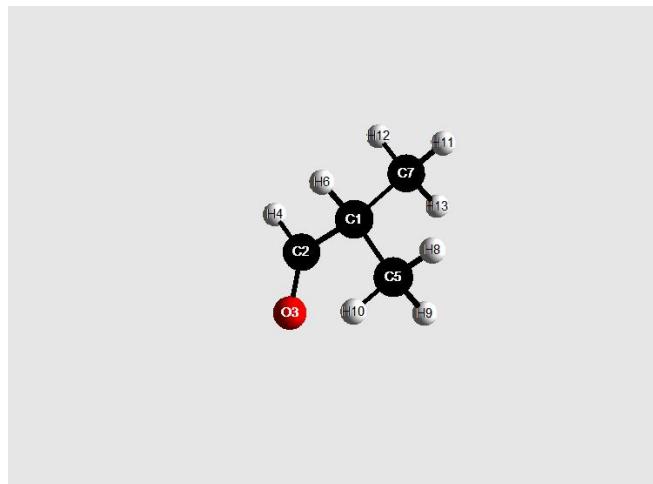
H3	O9	0.012084811602
H4	O9	0.012068501469
H5	O9	0.0039500447662
C6	O9	1.3115502926
H7	O9	0.018907420174
H8	O9	0.018924885671
C1	C1	0.0084890868496
C2	C1	0.049926516983
H3	C1	0.00054613729008
H4	C1	0.00054594915637
H5	C1	0.0017810629026
C6	C1	0.8889530272
H7	C1	0.0038971458243
H8	C1	0.0038967086675
O9	C1	0.12540115498

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.81586787159
C1	O3	0.08612358564
C2	O3	1.2206722741
C1	H4	0.03998875845
C2	H4	0.76792723005
O3	H4	0.092970414718
C1	C5	0.84615404063
C2	C5	0.02950378696
O3	C5	0.032184621791
H4	C5	0.0067737298045
C1	H6	0.80990126573
C2	H6	0.040138380451
O3	H6	0.014852595008
H4	H6	0.0035357649369
C5	H6	0.031114514043
C1	H7	0.80979321092
C2	H7	0.040131551505
O3	H7	0.014852685906
H4	H7	0.0035357118936
C5	H7	0.031082742628
H6	H7	0.032680675117
C1	H8	0.035602538148
C2	H8	0.0071300076099
O3	H8	0.0035286377727
H4	H8	0.0015614556232
C5	H8	0.83174104275
H6	H8	0.0030834913136
H7	H8	0.0030834915337
C1	H9	0.033424572906
C2	H9	0.0036918412734

O3	H9	0.013446896193
H4	H9	0.00062445932806
C5	H9	0.82340402599
H6	H9	0.0087220802225
H7	H9	0.0028017080937
H8	H9	0.03227828795
C1	C1	0.03346536412
C2	C1	0.0036897619173
O3	C1	0.013446941123
H4	C1	0.00062445153018
C5	C1	0.82350846959
H6	C1	0.0028017045781
H7	C1	0.0087221084163
H8	C1	0.032278215614
H9	C1	0.03199750404

## ISOBUTYRALDEHYDE



### HARTREE-FOCK

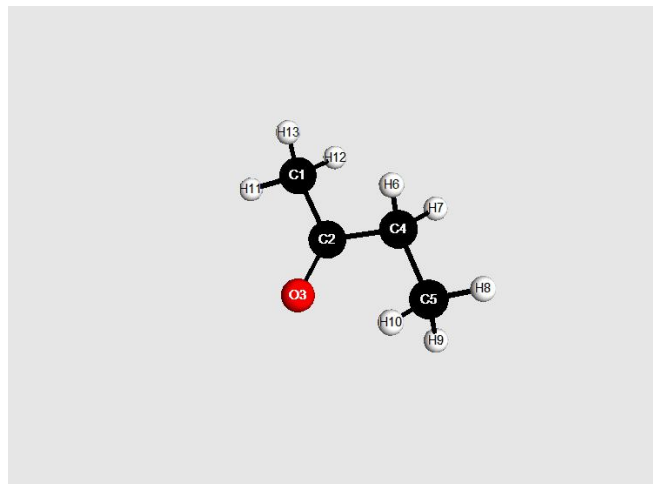
Atom A	Atom B	Delocalization index
C1	C2	0.92209908936
C1	O3	0.10884577513
C2	O3	1.305112647
C1	H4	0.047851577349
C2	H4	0.88277930892
O3	H4	0.12498343601
C1	C5	0.97135285197
C2	C5	0.035545556845
O3	C5	0.033127856938
H4	C5	0.0080945257082
C1	H6	0.93095393628
C2	H6	0.052518025496
O3	H6	0.018076255404
H4	H6	0.0036767644528
C5	H6	0.039166477214
C1	C7	0.96290197042
C2	C7	0.053209177637
O3	C7	0.017401953074
H4	C7	0.0084683795022
C5	C7	0.042696870606
H6	C7	0.04174807126
C1	H8	0.04316703014
C2	H8	0.0089252627926
O3	H8	0.0039474713135
H4	H8	0.0018627484469
C5	H8	0.96314013995
H6	H8	0.0036500087499
C7	H8	0.0075193680076
C1	H9	0.041024832214
C2	H9	0.0036411358193

O3	H9	0.011867019041
H4	H9	0.0005368077842
C5	H9	0.95550909671
H6	H9	0.01076700683
C7	H9	0.0070263848649
H8	H9	0.042010790132
C1	C1	0.040671890253
C2	C1	0.0036658546869
O3	C1	0.014764779956
H4	C1	0.00050794922829
C5	C1	0.95764861154
H6	C1	0.0033654992311
C7	C1	0.0098506729609
H8	C1	0.041107160547
H9	C1	0.04047771504
C1	H11	0.040785443608
C2	H11	0.010032161207
O3	H11	0.0034836860822
H4	H11	0.0010465393225
C5	H11	0.0069339094898
H6	H11	0.0043089956472
C7	H11	0.96069176758
H8	H11	0.0060368731751
H9	H11	0.00047078983781
C1	H11	0.00070351512601
C1	H12	0.040846861965
C2	H12	0.0083758259275
O3	H12	0.0021115113821
H4	H12	0.0086331464426
C5	H12	0.0098118935358
H6	H12	0.003554565014
C7	H12	0.9623698022
H8	H12	0.00073120885665
H9	H12	0.00072081262899
C1	H12	0.0023533581104
H11	H12	0.042044840553
C1	H13	0.040967756554
C2	H13	0.0053826684428
O3	H13	0.003001528413
H4	H13	0.00053528825522
C5	H13	0.007275747894
H6	H13	0.011089489069
C7	H13	0.96048534857
H8	H13	0.00051238280976
H9	H13	0.0057166479116
C1	H13	0.00076044599549
H11	H13	0.042040544675
H12	H13	0.042217706623





## ETHYL METHYL KETONE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.93153755398
C1	O3	0.12503192542
C2	O3	1.2646229678
C1	C4	0.050131833207
C2	C4	0.92217135166
O3	C4	0.11435108289
C1	C5	0.0071831754397
C2	C5	0.033337649705
O3	C5	0.034441456329
C4	C5	0.98242944283
C1	H6	0.007760723371
C2	H6	0.047027669283
O3	H6	0.017074740633
C4	H6	0.94477608656
C5	H6	0.038926309704
C1	H7	0.0077539394173
C2	H7	0.046992674143
O3	H7	0.017068808353
C4	H7	0.94473593481
C5	H7	0.038927463493
H6	H7	0.042141882469
C1	H8	0.0013942733127
C2	H8	0.0090611401893
O3	H8	0.0042165135072
C4	H8	0.045420865522
C5	H8	0.96711756261
H6	H8	0.0036693681443
H7	H8	0.0036703174332
C1	H9	0.00055262154946
C2	H9	0.0034397641719

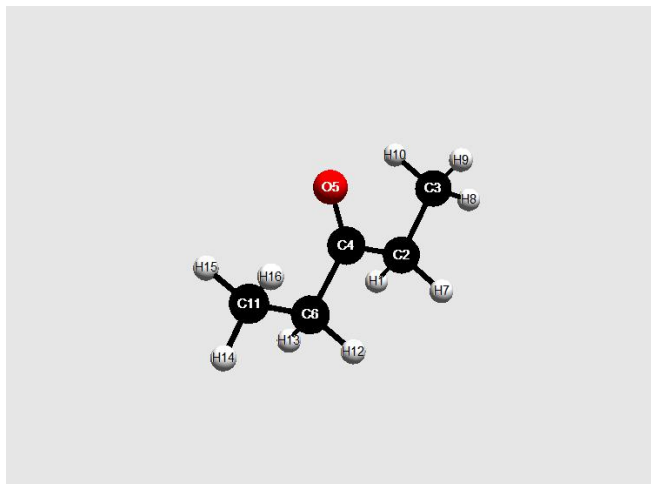
O3	H9	0.013667050261
C4	H9	0.042232209308
C5	H9	0.95855329867
H6	H9	0.010835560596
H7	H9	0.0033108585311
H8	H9	0.041830801959
C1	C1	0.00055263801531
C2	C1	0.003425508163
O3	C1	0.013679761523
C4	C1	0.042229371192
C5	C1	0.95858607321
H6	C1	0.0033120893029
H7	C1	0.010835092431
H8	C1	0.041829208964
H9	C1	0.040927732638
C1	H11	0.95815435924
C2	H11	0.034864610348
O3	H11	0.021228713527
C4	H11	0.0079945945545
C5	H11	0.0017266078646
H6	H11	0.00079442537966
H7	H11	0.000797364266
H8	H11	0.00039890145461
H9	H11	5.5483294481e-05
C1	H11	5.5512973164e-05
C1	H12	0.96075717733
C2	H12	0.043906074296
O3	H12	0.018079717759
C4	H12	0.0065207037772
C5	H12	0.00066464677211
H6	H12	0.00064390594339
H7	H12	0.0063298161897
H8	H12	5.2279420778e-05
H9	H12	8.7648693254e-05
C1	H12	0.00021680982397
H11	H12	0.037749885474
C1	H13	0.96085184574
C2	H13	0.043884396537
O3	H13	0.018070954412
C4	H13	0.006545079989
C5	H13	0.00066700671564
H6	H13	0.0063347404043
H7	H13	0.00064435019786
H8	H13	5.2352281614e-05
H9	H13	0.00021701541419
C1	H13	8.7629569625e-05
H11	H13	0.037750252173
H12	H13	0.041638774003

## CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.79555406279
C1	O3	0.092483262845
C2	O3	1.1853734866
C1	C4	0.041119848221
C2	C4	0.81037499056
O3	C4	0.096759130312
C1	H5	0.81074539358
C2	H5	0.029491854945
O3	H5	0.020788090798
C4	H5	0.005554400897
C1	C6	0.83573186271
C2	C6	0.040521425282
O3	C6	0.018258704131
C4	C6	0.0049025540139
H5	C6	0.03144469407
C1	H7	0.8156903017
C2	H7	0.031077945196
O3	H7	0.011515108486
C4	H7	0.010308099466
H5	H7	0.029764311361
C6	H7	0.033191169461
C1	H8	0.033967715111
C2	H8	0.0076435336644
O3	H8	0.0032010191722
C4	H8	0.00084059294742
H5	H8	0.0031075877766
C6	H8	0.82920673826
H7	H8	0.0034005753079
C1	H9	0.032764762145
C2	H9	0.0052006052174
O3	H9	0.0083207273017
C4	H9	0.0004673425632
H5	H9	0.0030851198985
C6	H9	0.82525124659
H7	H9	0.0087318223359
H8	H9	0.032128927615
C1	C1	0.033444025217
C2	C1	0.0047428714807
O3	C1	0.0011401076155
C4	C1	0.0052869537025
H5	C1	0.0086719316837
C6	C1	0.82631157291
H7	C1	0.0029048392018
H8	C1	0.033067434501
H9	C1	0.032634824981
C1	H11	0.0065239203945

C2	H11	0.027420456458
O3	H11	0.020180927069
C4	H11	0.82370934405
H5	H11	0.0014375574292
C6	H11	0.00048931143201
H7	H11	0.0011810006971
H8	H11	0.00014773505743
H9	H11	4.643696211e-05
C1	H11	0.00044361507023
C1	H12	0.0043269456066
C2	H12	0.035438502512
O3	H12	0.015032426974
C4	H12	0.82340390792
H5	H12	0.00032631007625
C6	H12	0.00076669546131
H7	H12	0.005231196554
H8	H12	9.6563179684e-05
H9	H12	0.00018089830102
C1	H12	0.00047357275969
H11	H12	0.029431051407
C1	H13	0.0052776879214
C2	H13	0.032020821785
O3	H13	0.013780576683
C4	H13	0.82298012888
H5	H13	0.00062452463991
C6	H13	0.0054190453847
H7	H13	0.0022543789506
H8	H13	0.0006207804286
H9	H13	0.00037696998298
C1	H13	0.010958973637
H11	H13	0.029250091368
H12	H13	0.03224142612

## DIETHYL KETONE



### HARTREE-FOCK

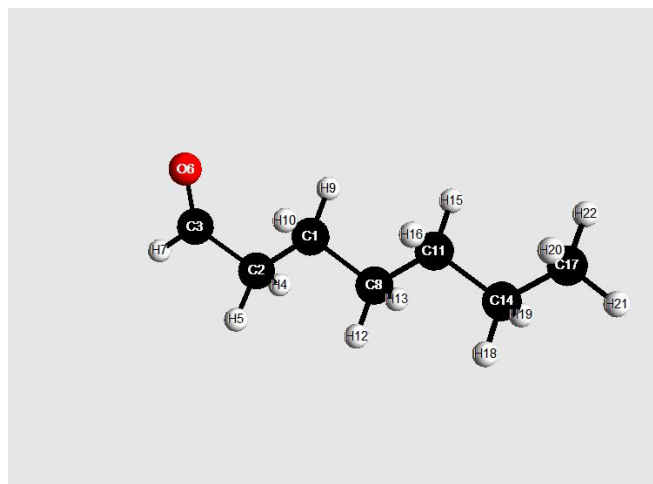
Atom A	Atom B	Delocalization index
H1	C2	0.94466673393
H1	C3	0.039033728651
C2	C3	0.98224541298
H1	C4	0.046568841004
C2	C4	0.92089621437
C3	C4	0.033344826854
H1	O5	0.016857356372
C2	O5	0.11400559667
C3	O5	0.034677401778
C4	O5	1.2601639717
H1	C6	0.0075326106123
C2	C6	0.048851316095
C3	C6	0.0069016380746
C4	C6	0.92111839568
O5	C6	0.11430040938
H1	H7	0.042142891632
C2	H7	0.94485339119
C3	H7	0.039057477596
C4	H7	0.046422385798
O5	H7	0.016758495353
C6	H7	0.0076904192926
H1	H8	0.0036864173486
C2	H8	0.045399701564
C3	H8	0.9671200609
C4	H8	0.0090804373659
O5	H8	0.0042426601001
C6	H8	0.0013427360295
H7	H8	0.0036905210978
H1	H9	0.010833277936
C2	H9	0.042230764199

C3	H9	0.95866112065
C4	H9	0.003436943609
O5	H9	0.013682602539
C6	H9	0.00053123491099
H7	H9	0.003321728401
H8	H9	0.041918948805
H1	H1	0.0033316472028
C2	H1	0.042113286131
C3	H1	0.95853356769
C4	H1	0.003408000029
O5	H1	0.013945084569
C6	H1	0.0005411539464
H7	H1	0.010824162278
H8	H1	0.041878050428
H9	H1	0.041004799369
H1	C11	0.00075315650243
C2	C11	0.0069011230229
C3	C11	0.0014888719285
C4	C11	0.033403294012
O5	C11	0.034716506666
C6	C11	0.98259271521
H7	C11	0.00079022892078
H8	C11	0.00033025504533
H9	C11	5.9677465371e-05
H1	C11	6.0287297249e-05
H1	H12	0.00074491357366
C2	H12	0.007520746627
C3	H12	0.00075223897473
C4	H12	0.046643935123
O5	H12	0.016868089762
C6	H12	0.94474668153
H7	H12	0.0075612473376
H8	H12	4.289430372e-05
H9	H12	8.5974346063e-05
H1	H12	0.00024292254224
C11	H12	0.039063125482
H1	H13	0.0075781039949
C2	H13	0.0076857914216
C3	H13	0.00079074373221
C4	H13	0.04636430991
O5	H13	0.016750490878
C6	H13	0.94494466178
H7	H13	0.00076090911032
H8	H13	4.4091772892e-05
H9	H13	0.00024532077888
H1	H13	8.5888152728e-05
C11	H13	0.039058011137
H12	H13	0.042144952983

H1	H14	4.2947118176e-05
C2	H14	0.0013423778629
C3	H14	0.00033026855763
C4	H14	0.0090836932542
O5	H14	0.0042434883834
C6	H14	0.04542973062
H7	H14	4.4034306134e-05
H8	H14	0.00010664453549
H9	H14	1.3044310933e-05
H1	H14	1.3012218305e-05
C11	H14	0.96716269765
H12	H14	0.0036885656018
H13	H14	0.0036891881253
H1	H15	8.5998070829e-05
C2	H15	0.00053036472481
C3	H15	5.9566307016e-05
C4	H15	0.0034518269383
O5	H15	0.013655807176
C6	H15	0.042229041513
H7	H15	0.00024509594595
H8	H15	1.3026768734e-05
H9	H15	1.0938149153e-05
H1	H15	9.6754188493e-06
C11	H15	0.95879784591
H12	H15	0.010835642287
H13	H15	0.0033226248564
H14	H15	0.041924509969
H1	H16	0.00024313742813
C2	H16	0.00054117228768
C3	H16	6.0369638934e-05
C4	H16	0.0034064406819
O5	H16	0.013975967442
C6	H16	0.042198942663
H7	H16	8.5872484609e-05
H8	H16	1.3027188187e-05
H9	H16	9.7060171567e-06
H1	H16	1.1240103678e-05
C11	H16	0.95865734707
H12	H16	0.0033305768098
H13	H16	0.010824342197
H14	H16	0.041873540196
H15	H16	0.041005691901



## HEPTANAL



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.96805735649
C1	C3	0.033752147229
C2	C3	0.93860879794
C1	H4	0.0365678829
C2	H4	0.94045376905
C3	H4	0.051932539184
C1	H5	0.036546178293
C2	H5	0.94033829457
C3	H5	0.051937277096
H4	H5	0.042285921515
C1	O6	0.028842864529
C2	O6	0.11197766769
C3	O6	1.3115051518
H4	O6	0.018548565827
H5	O6	0.018551509095
C1	H7	0.008158454328
C2	H7	0.049979817277
C3	H7	0.88888724652
H4	H7	0.0039121638322
H5	H7	0.003910325079
O6	H7	0.12570286706
C1	C8	0.9661661839
C2	C8	0.045651981433
C3	C8	0.0079297077215
H4	C8	0.0070977292229
H5	C8	0.0070900859052
O6	C8	0.003510146441
H7	C8	0.0014309000887
C1	H9	0.94173087519
C2	H9	0.042959056378

C3	H9	0.0036899338489
H4	H9	0.0032631697851
H5	H9	0.010537907005
O6	H9	0.013445759791
H7	H9	0.00047589198165
C8	H9	0.039200240969
C1	C1	0.94162244827
C2	C1	0.04292714305
C3	C1	0.0036892753015
H4	C1	0.010538419544
H5	C1	0.0032699404074
O6	C1	0.013421859658
H7	C1	0.00047549670717
C8	C1	0.039202336363
H9	C1	0.04100481106
C1	C11	0.042504295884
C2	C11	0.0090806146779
C3	C11	0.0014628686002
H4	C11	0.00075960651704
H5	C11	0.00075832015987
O6	C11	0.00022552363404
H7	C11	0.0004674083306
C8	C11	0.96544914576
H9	C11	0.0073715677759
C1	C11	0.0073758386582
C1	H12	0.042107514025
C2	H12	0.0079923893628
C3	H12	0.00064314510547
H4	H12	0.00055264623067
H5	H12	0.0067592507316
O6	H12	0.00066933093764
H7	H12	6.3957825433e-05
C8	H12	0.94439684422
H9	H12	0.010746628114
C1	H12	0.0035139214251
C11	H12	0.041270456146
C1	H13	0.042104018929
C2	H13	0.0079940404302
C3	H13	0.00064259255201
H4	H13	0.0067651946843
H5	H13	0.00055161247769
O6	H13	0.00066880281749
H7	H13	6.3827641414e-05
C8	H13	0.94427847518
H9	H13	0.0035160664327
C1	H13	0.010747205833
C11	H13	0.041321227262
H12	H13	0.044685797992

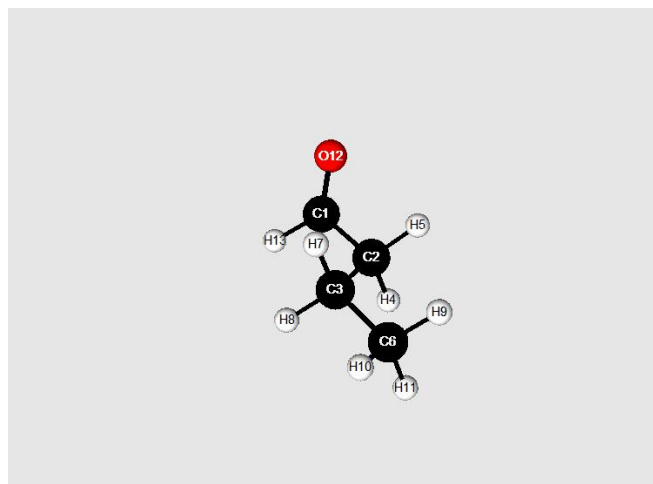
C1	C14	0.0088543890811
C2	C14	0.0015423287932
C3	C14	0.00028503497322
H4	C14	4.7208686934e-05
H5	C14	4.717941468e-05
O6	C14	5.9402260239e-05
H7	C14	0.00010548798312
C8	C14	0.042494995446
H9	C14	0.00079638023563
C1	C14	0.00079706421774
C11	C14	0.96562569699
H12	C14	0.0076802474631
H13	C14	0.0076842816215
C1	H15	0.0077466988022
C2	H15	0.00082170727973
C3	H15	4.8918265331e-05
H4	H15	4.5334327283e-05
H5	H15	0.00035968782941
O6	H15	3.9908158314e-05
H7	H15	1.493995084e-05
C8	H15	0.041721328547
H9	H15	0.0071286242888
C1	H15	0.00057348028987
C11	H15	0.94384669811
H12	H15	0.011029254783
H13	H15	0.0036440414158
C14	H15	0.041348196352
C1	H16	0.0077515647012
C2	H16	0.00082108052786
C3	H16	4.8912674465e-05
H4	H16	0.00035980432533
H5	H16	4.5299931335e-05
O6	H16	3.9864905492e-05
H7	H16	1.4939724898e-05
C8	H16	0.04176060042
H9	H16	0.00057279445316
C1	H16	0.0071271192106
C11	H16	0.94373109386
H12	H16	0.0036500092871
H13	H16	0.011029403606
C14	H16	0.041345510864
H15	H16	0.044100053299
C1	C17	0.0015410986387
C2	C17	0.00031032097248
C3	C17	8.5001794776e-05
H4	C17	1.349615466e-05
H5	C17	1.3473211761e-05
O6	C17	1.6801779649e-05

H7	C17	2.8175559889e-05
C8	C17	0.0091476532974
H9	C17	4.8942118945e-05
C1	C17	4.8993871311e-05
C11	C17	0.044289737682
H12	C17	0.00085260166383
H13	C17	0.00085392063227
C14	C17	0.9775834358
H15	C17	0.0079808124618
H16	C17	0.0079904733636
C1	H18	0.00083815698028
C2	H18	5.086814332e-05
C3	H18	1.0334888336e-05
H4	H18	4.6102161947e-06
H5	H18	1.7101848559e-05
O6	H18	1.0810036072e-05
H7	H18	2.2931252728e-06
C8	H18	0.0076447280457
H9	H18	0.00038532103521
C1	H18	4.8958722911e-05
C11	H18	0.04216534719
H12	H18	0.0075018895273
H13	H18	0.00061162505192
C14	H18	0.94838463145
H15	H18	0.011201137243
H16	H18	0.0036693073154
C17	H18	0.043845890352
C1	H19	0.00083781408698
C2	H19	5.085104969e-05
C3	H19	1.0328064388e-05
H4	H19	1.7120014114e-05
H5	H19	4.6045444367e-06
O6	H19	1.0792514167e-05
H7	H19	2.2925787155e-06
C8	H19	0.0076409135269
H9	H19	4.8944719133e-05
C1	H19	0.0003853609538
C11	H19	0.042184572751
H12	H19	0.00061087731258
H13	H19	0.007505042425
C14	H19	0.94825026831
H15	H19	0.0036705002617
H16	H19	0.011201399176
C17	H19	0.043853194212
H18	H19	0.044515206802
C1	C2	5.9900449608e-05
C2	C2	1.4722854526e-05
C3	C2	3.5083007749e-06

H4	C2	3.1448367675e-06
H5	C2	8.5421059116e-07
O6	C2	2.7164851604e-06
H7	C2	1.0476108953e-06
C8	C2	0.00077424628159
H9	C2	4.5779135901e-06
C1	C2	1.7394290868e-05
C11	C2	0.0071185683785
H12	C2	4.9746925782e-05
H13	C2	0.00038439952051
C14	C2	0.041721727761
H15	C2	0.00056347807475
H16	C2	0.0067104112391
C17	C2	0.96293955209
H18	C2	0.0037008421684
H19	C2	0.011569213699
C1	H21	0.00036819099769
C2	H21	0.00011566540621
C3	H21	2.7332962997e-05
H4	H21	3.4185992823e-06
H5	H21	3.4141317984e-06
O6	H21	5.6822053984e-06
H7	H21	1.0555545511e-05
C8	H21	0.0018826302539
H9	H21	1.3828494868e-05
C1	H21	1.3847458546e-05
C11	H21	0.010351292608
H12	H21	5.1277699969e-05
H13	H21	5.1304913381e-05
C14	H21	0.042338675551
H15	H21	0.00086213361967
H16	H21	0.00086307060242
C17	H21	0.96674339315
H18	H21	0.003905353779
H19	H21	0.0039125544376
C2	H21	0.04436295249
C1	H22	5.991214045e-05
C2	H22	1.4738178608e-05
C3	H22	3.5110555713e-06
H4	H22	8.5489609384e-07
H5	H22	3.1449420899e-06
O6	H22	2.7190043859e-06
H7	H22	1.0481944031e-06
C8	H22	0.0007755934964
H9	H22	1.7408968725e-05
C1	H22	4.5843661083e-06
C11	H22	0.007134281105
H12	H22	0.00038449033084

H13	H22	4.9781009409e-05
C14	H22	0.041690975568
H15	H22	0.0067174032255
H16	H22	0.00056436709063
C17	H22	0.96288107216
H18	H22	0.011570044807
H19	H22	0.0036935885894
C2	H22	0.044856111356
H21	H22	0.044362641899

## BUTANAL



## HARTREE-FOCK

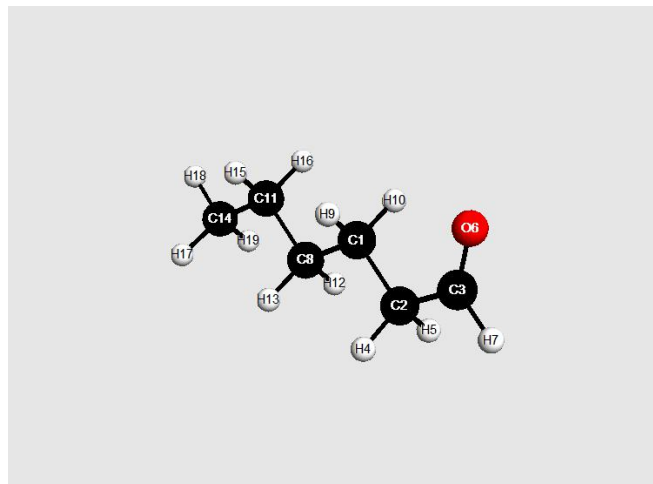
Atom A	Atom B	Delocalization index
C1	C2	0.93322863205
C1	C3	0.047873362032
C2	C3	0.96222793506
C1	H4	0.04986904526
C2	H4	0.94268635258
C3	H4	0.038882977163
C1	H5	0.037047741075
C2	H5	0.94341499941
C3	H5	0.036089007753
H4	H5	0.038242484605
C1	C6	0.0093022975115
C2	C6	0.045786716662
C3	C6	0.97761766224
H4	C6	0.0082995356213
H5	C6	0.0066506060367
C1	H7	0.0057786270909
C2	H7	0.043682519065
C3	H7	0.95049947072
H4	H7	0.011055590815
H5	H7	0.0034401799172
C6	H7	0.042180222676
C1	H8	0.007764833732
C2	H8	0.04349341449
C3	H8	0.94927632983
H4	H8	0.0034709479514
H5	H8	0.010496272118
C6	H8	0.042735669963
H7	H8	0.042871146867
C1	H9	0.00074974684728
C2	H9	0.0073519784903

C3	H9	0.042042183161
H4	H9	0.00053464460538
H5	H9	0.0055121707065
C6	H9	0.96244117025
H7	H9	0.0035452623049
H8	H9	0.01133757411
C1	C1	0.0018807573112
C2	C1	0.010522493775
C3	C1	0.04245409796
H4	C1	0.00088131314112
H5	C1	0.00069054009525
C6	C1	0.96558271596
H7	C1	0.0037836292581
H8	C1	0.0037850926112
H9	C1	0.0432715371
C1	H11	0.00071525074317
C2	H11	0.0073457912084
C3	H11	0.042340564574
H4	H11	0.0063835403322
H5	H11	0.00046043047235
C6	H11	0.96258892853
H7	H11	0.011390928615
H8	H11	0.0036974119947
H9	H11	0.044023767424
C1	H11	0.043410856958
C1	O12	1.3162970241
C2	O12	0.1175307335
C3	O12	0.01770390702
H4	O12	0.018948313297
H5	O12	0.020584707102
C6	O12	0.0029275344798
H7	O12	0.0035447544394
H8	O12	0.0020367861009
H9	O12	0.00016405577746
C1	O12	0.00081576969774
H11	O12	0.0004224960706
C1	H13	0.88500249439
C2	H13	0.04832776128
C3	H13	0.0067023140441
H4	H13	0.0031606960322
H5	H13	0.0093000294483
C6	H13	0.001027200956
H7	H13	0.00057074942372
H8	H13	0.0073880487173
H9	H13	0.00038149448866
C1	H13	0.00010376726693
H11	H13	6.1048876222e-05
O12	H13	0.12587365965





## HEXANAL



## HARTREE-FOCK

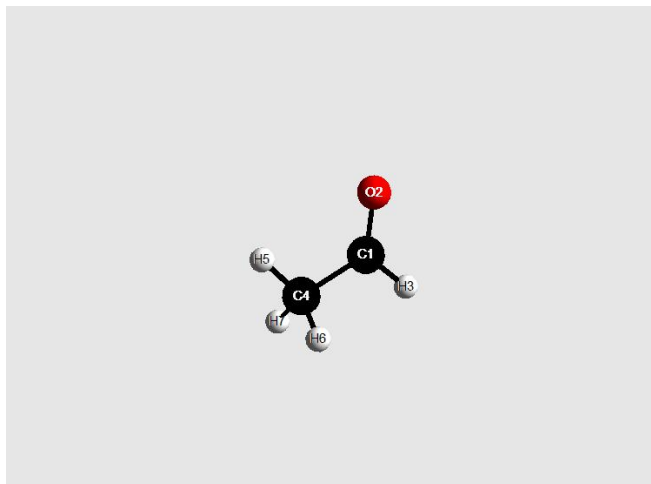
Atom A	Atom B	Delocalization index
C1	C2	0.96811600605
C1	C3	0.033785953006
C2	C3	0.9387006461
C1	H4	0.03660989214
C2	H4	0.94042552938
C3	H4	0.051920774093
C1	H5	0.036555071855
C2	H5	0.94043805781
C3	H5	0.051928953318
H4	H5	0.042277212214
C1	O6	0.028896183799
C2	O6	0.11203331013
C3	O6	1.311693148
H4	O6	0.018551663529
H5	O6	0.018551506425
C1	H7	0.0081608845168
C2	H7	0.049999381933
C3	H7	0.88890183474
H4	H7	0.0039106555963
H5	H7	0.0039111425473
O6	H7	0.1256833559
C1	C8	0.96638943645
C2	C8	0.045661136181
C3	C8	0.0079310133902
H4	C8	0.0070882397021
H5	C8	0.0070971573332
O6	C8	0.0035128849125
H7	C8	0.0014315184823
C1	H9	0.94178813416
C2	H9	0.042918969372

C3	H9	0.0036898848209
H4	H9	0.0032669047454
H5	H9	0.010538905467
O6	H9	0.013428801931
H7	H9	0.00047615413723
C8	H9	0.039240872664
C1	C1	0.94164311939
C2	C1	0.042949981459
C3	C1	0.0036895854613
H4	C1	0.010538871296
H5	C1	0.0032666720017
O6	C1	0.013429018002
H7	C1	0.00047614438475
C8	C1	0.039215356693
H9	C1	0.041003489903
C1	C11	0.042408685265
C2	C11	0.0090725592219
C3	C11	0.0014617604864
H4	C11	0.00075993374931
H5	C11	0.00076037532224
O6	C11	0.00022662491531
H7	C11	0.00046694832863
C8	C11	0.96534675695
H9	C11	0.0073643363439
C1	C11	0.0073536758964
C1	H12	0.042065514532
C2	H12	0.0079797407013
C3	H12	0.00064071913819
H4	H12	0.00055109896936
H5	H12	0.0067443173235
O6	H12	0.00066974561858
H7	H12	6.3808909705e-05
C8	H12	0.94441526056
H9	H12	0.010759347118
C1	H12	0.003513100479
C11	H12	0.041458180111
C1	H13	0.042132650866
C2	H13	0.0079824360305
C3	H13	0.00064084837976
H4	H13	0.006745144964
H5	H13	0.00055116995037
O6	H13	0.00066979655539
H7	H13	6.3832894826e-05
C8	H13	0.94426617404
H9	H13	0.0035121621182
C1	H13	0.010759451701
C11	H13	0.041446448743
H12	H13	0.044722567857

C1	C14	0.0091272618869
C2	C14	0.0015883568951
C3	C14	0.00029557411722
H4	C14	4.9319641363e-05
H5	C14	4.9317295695e-05
O6	C14	6.2256341218e-05
H7	C14	0.00010888449312
C8	C14	0.044555011382
H9	C14	0.00081080361183
C1	C14	0.00081066648062
C11	C14	0.97775766792
H12	C14	0.0080533577053
H13	C14	0.0080515607511
C1	H15	0.0077215075854
C2	H15	0.00082592616497
C3	H15	4.945877059e-05
H4	H15	4.5328394407e-05
H5	H15	0.00036064672913
O6	H15	4.2217552737e-05
H7	H15	1.541795426e-05
C8	H15	0.042191185768
H9	H15	0.0070983486055
C1	H15	0.00057151113073
C11	H15	0.94812879383
H12	H15	0.011205845351
H13	H15	0.0036752080316
C14	H15	0.043553393057
C1	H16	0.0077197525748
C2	H16	0.00082605523563
C3	H16	4.9460827201e-05
H4	H16	0.00036065612799
H5	H16	4.5326497172e-05
O6	H16	4.2219732895e-05
H7	H16	1.5418755339e-05
C8	H16	0.04216334441
H9	H16	0.00057158571672
C1	H16	0.0070980425713
C11	H16	0.94799141434
H12	H16	0.0036745558544
H13	H16	0.011205927901
C14	H16	0.043556034355
H15	H16	0.043996095719
C1	H17	0.00078477098941
C2	H17	6.2290983836e-05
C3	H17	1.2040634127e-05
H4	H17	1.747137968e-05
H5	H17	4.4823320107e-06
O6	H17	1.0492425141e-05

H7	H17	3.2399849718e-06
C8	H17	0.0071283378782
H9	H17	4.7104452642e-05
C1	H17	0.00037314625904
C11	H17	0.041787229142
H12	H17	0.00057041981782
H13	H17	0.0067720495977
C14	H17	0.96307095875
H15	H17	0.0036820965985
H16	H17	0.011536191326
C1	H18	0.0018559835786
C2	H18	0.00038151409506
C3	H18	0.00010695380991
H4	H18	1.4083350956e-05
H5	H18	1.4083387093e-05
O6	H18	2.1323416394e-05
H7	H18	3.5366503808e-05
C8	H18	0.010364514315
H9	H18	4.9116185711e-05
C1	H18	4.9115113198e-05
C11	H18	0.042182469119
H12	H18	0.00087361752456
H13	H18	0.00087362783996
C14	H18	0.96639622615
H15	H18	0.0038702302683
H16	H18	0.0038712426733
H17	H18	0.044323605201
C1	H19	0.00078510047448
C2	H19	6.2284779888e-05
C3	H19	1.2044489069e-05
H4	H19	4.4830526315e-06
H5	H19	1.7475246462e-05
O6	H19	1.049469497e-05
H7	H19	3.2403432617e-06
C8	H19	0.0071404507623
H9	H19	0.00037320010043
C1	H19	4.7111436016e-05
C11	H19	0.041801249112
H12	H19	0.0067740674373
H13	H19	0.00057050304157
C14	H19	0.96308150675
H15	H19	0.011536383607
H16	H19	0.0036812949706
H17	H19	0.044992769046
H18	H19	0.044323664505

## ACETALDEHYDE



### HARTREE-FOCK

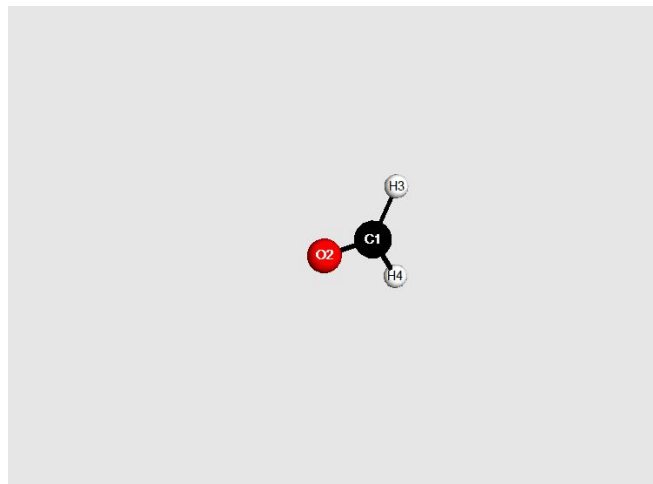
Atom A	Atom B	Delocalization index
C1	O2	1.3130845882
C1	H3	0.88846294786
O2	H3	0.12593363207
C1	C4	0.94900733597
O2	C4	0.12346539626
H3	C4	0.050413791328
C1	H5	0.036528191666
O2	H5	0.018994172412
H3	H5	0.0097973367927
C4	H5	0.95892616123
C1	H6	0.048081108348
O2	H6	0.01978543283
H3	H6	0.0032434743867
C4	H6	0.95999202852
H5	H6	0.037258113249
C1	H7	0.048084112348
O2	H7	0.019785453111
H3	H7	0.0032434591698
C4	H7	0.95996480532
H5	H7	0.037258019431
H6	H7	0.040866084843

### CCSD

Atom A	Atom B	Delocalization index
C1	O2	1.2267879108
C1	H3	0.76810100126
O2	H3	0.093837385573
C1	C4	0.82780145501
O2	C4	0.094924885562
H3	C4	0.040859200554

C1	H5	0.028944914543
O2	H5	0.018970060247
H3	H5	0.0082040250611
C4	H5	0.8241241117
C1	H6	0.037102417358
O2	H6	0.015516151187
H3	H6	0.0030399655097
C4	H6	0.82535068902
H5	H6	0.029205868114
C1	H7	0.037099378201
O2	H7	0.015516191791
H3	H7	0.0030399072983
C4	H7	0.82540854905
H5	H7	0.029205750793
H6	H7	0.03219956526

## FORMALDEHYDE



### HARTREE-FOCK

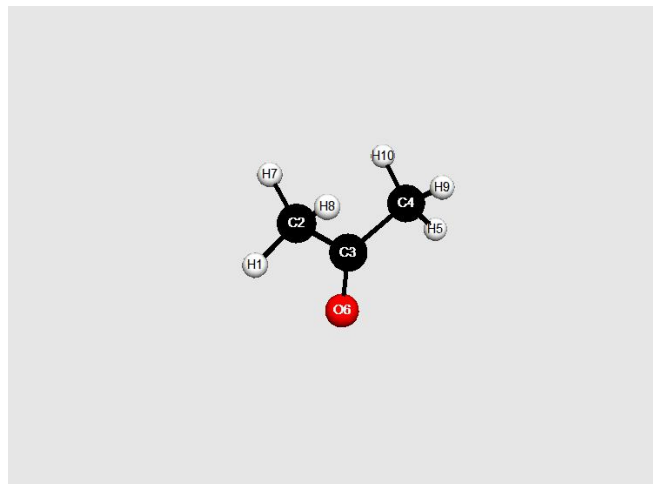
Atom A	Atom B	Delocalization index
C1	O2	1.3790605198
C1	H3	0.89799032154
O2	H3	0.12366100364
C1	H4	0.89800781294
O2	H4	0.12366118646
H3	H4	0.051065704385

### CCSD

Atom A	Atom B	Delocalization index
C1	O2	1.2708393877
C1	H3	0.77791292086
O2	H3	0.09135772778
C1	H4	0.77791732583
O2	H4	0.091357747811
H3	H4	0.040567849341



## DIMETHYL KETONE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	C2	0.95815174929
H1	C3	0.034763198405
C2	C3	0.9324659071
H1	C4	0.0083026787698
C2	C4	0.051261890499
C3	C4	0.93230026174
H1	H5	0.0019861849541
C2	H5	0.0082992419401
C3	H5	0.034728342779
C4	H5	0.95829010583
H1	O6	0.021023212796
C2	O6	0.12526250431
C3	O6	1.2686877879
C4	O6	0.12521064168
H5	O6	0.020958889244
H1	H7	0.037610107782
C2	H7	0.9607464651
C3	H7	0.044290186938
C4	H7	0.0065910019256
H5	H7	0.0006645347904
O6	H7	0.018329607296
H1	H8	0.037627376138
C2	H8	0.96070534948
C3	H8	0.044276021467
C4	H8	0.0066444049352
H5	H8	0.00068910306623
O6	H8	0.018327824754
H7	H8	0.041600392805
H1	H9	0.00065944499946
C2	H9	0.0065037486687

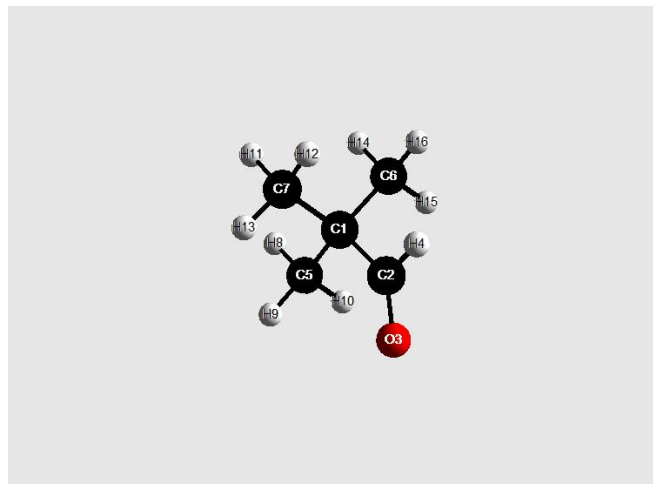
C3	H9	0.044447958897
C4	H9	0.96055872205
H5	H9	0.037622941807
O6	H9	0.018401894626
H7	H9	0.00054749484171
H8	H9	0.0052012992917
H1	H1	0.00069588681549
C2	H1	0.006740745849
C3	H1	0.044123458814
C4	H1	0.96080619273
H5	H1	0.037616864161
O6	H1	0.018231620753
H7	H1	0.0053367783502
H8	H1	0.00054864592525
H9	H1	0.041593606139

### CCSD

Atom A	Atom B	Delocalization index
H1	C2	0.82364674094
H1	C3	0.027351125434
C2	C3	0.81062837905
H1	C4	0.0067928158705
C2	C4	0.043688438869
C3	C4	0.81037779764
H1	H5	0.0018416930879
C2	H5	0.0068007048853
C3	H5	0.02730411536
C4	H5	0.8235939327
H1	O6	0.020512270264
C2	O6	0.096257917139
C3	O6	1.1908044341
C4	O6	0.096209065593
H5	O6	0.02051202675
H1	H7	0.029417361568
C2	H7	0.82511143468
C3	H7	0.03397793624
C4	H7	0.0060793657055
H5	H7	0.00060113143955
O6	H7	0.014384817196
H1	H8	0.029420321406
C2	H8	0.82529803225
C3	H8	0.033901611035
C4	H8	0.0061792006472
H5	H8	0.00062245289226
O6	H8	0.014357012306
H7	H8	0.032640420964
H1	H9	0.00059940882362
C2	H9	0.0060757385143

C3	H9	0.034020615973
C4	H9	0.825033107
H5	H9	0.029424826649
O6	H9	0.014404930805
H7	H9	0.00050730731201
H8	H9	0.0055662904808
H1	H1	0.00062424187843
C2	H1	0.0062282019766
C3	H1	0.033843806592
C4	H1	0.82523617359
H5	H1	0.029413503694
O6	H1	0.014337042714
H7	H1	0.0056204876038
H8	H1	0.00051569119157
H9	H1	0.032640861238

## PIVALDEHYDE



## HARTREE-FOCK

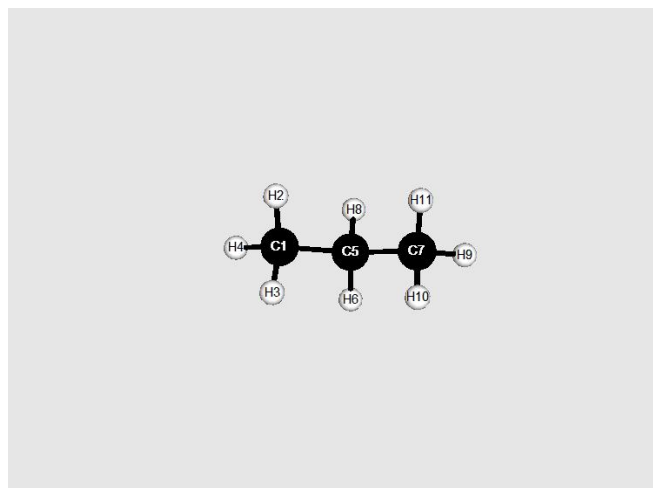
Atom A	Atom B	Delocalization index
C1	C2	0.90584702489
C1	O3	0.10453246003
C2	O3	1.3013679738
C1	H4	0.046532769125
C2	H4	0.87746700158
O3	H4	0.12417883438
C1	C5	0.95873964315
C2	C5	0.035280814401
O3	C5	0.034497629707
H4	C5	0.0078037452263
C1	C6	0.95034047737
C2	C6	0.054758620083
O3	C6	0.017150351835
H4	C6	0.0082434950859
C5	C6	0.043836093404
C1	C7	0.95033280284
C2	C7	0.054728288184
O3	C7	0.017146183256
H4	C7	0.0082396196302
C5	C7	0.043775131066
C6	C7	0.045533649809
C1	H8	0.0413608193
C2	H8	0.0087572130131
O3	H8	0.0039577041546
H4	H8	0.0019600979843
C5	H8	0.95897453715
C6	H8	0.0076427873558
C7	H8	0.0076381051378
C1	H9	0.038956606281
C2	H9	0.0034849583543

O3	H9	0.014187780385
H4	H9	0.00048714656334
C5	H9	0.9539151348
C6	H9	0.0096172105113
C7	H9	0.0074829817909
H8	H9	0.041333386674
C1	C1	0.038881657398
C2	C1	0.003489263804
O3	C1	0.014188224146
H4	C1	0.00048715276271
C5	C1	0.95405612078
C6	C1	0.0074965192566
C7	C1	0.0096152641039
H8	C1	0.041333293239
H9	C1	0.039925446061
C1	H11	0.039044505527
C2	H11	0.010226761794
O3	H11	0.0037971079836
H4	H11	0.0010314266812
C5	H11	0.0070264455754
C6	H11	0.0084585041233
C7	H11	0.95533723143
H8	H11	0.0061165267388
H9	H11	0.00047053094697
C1	H11	0.00070671316106
C1	H12	0.039062380856
C2	H12	0.0082529226362
O3	H12	0.0019928343088
H4	H12	0.0082135848801
C5	H12	0.0096277398535
C6	H12	0.0075816787433
C7	H12	0.95840456307
H8	H12	0.00073581943052
H9	H12	0.0007092957761
C1	H12	0.0025634412912
H11	H12	0.042087561256
C1	H13	0.039002620751
C2	H13	0.00562202132
O3	H13	0.0034622536531
H4	H13	0.00050723398261
C5	H13	0.0077872132005
C6	H13	0.0099645334229
C7	H13	0.95976761438
H8	H13	0.00052257745579
H9	H13	0.0064794992763
C1	H13	0.00075386602253
H11	H13	0.041404276256
H12	H13	0.04169845153

C1	H14	0.039047812018
C2	H14	0.010230606295
O3	H14	0.0037971229953
H4	H14	0.0010315425025
C5	H14	0.0070173890267
C6	H14	0.95536378877
C7	H14	0.0084583541125
H8	H14	0.0061169168103
H9	H14	0.0007067463517
C1	H14	0.00047051288603
H11	H14	0.0068648837709
H12	H14	0.00055420410022
H13	H14	0.00077564846116
C1	H15	0.03897456577
C2	H15	0.0056208378546
O3	H15	0.0034623897127
H4	H15	0.0005072804662
C5	H15	0.0078228717367
C6	H15	0.95985113286
C7	H15	0.009966842415
H8	H15	0.00052260933836
H9	H15	0.00075390960154
C1	H15	0.0064794133567
H11	H15	0.00077562549268
H12	H15	0.00074764493734
H13	H15	0.0026098442752
H14	H15	0.041403504974
C1	H16	0.039066190892
C2	H16	0.0082702109106
O3	H16	0.0019926851827
H4	H16	0.0082133110935
C5	H16	0.0096299053872
C6	H16	0.95837275221
C7	H16	0.0075950192244
H8	H16	0.00073586433875
H9	H16	0.002563441861
C1	H16	0.00070925720409
H11	H16	0.00055418508208
H12	H16	0.0065999695205
H13	H16	0.00074763237308
H14	H16	0.0420872053
H15	H16	0.041697715349

# ALKANES

## PROPANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	H2	0.96306860574
C1	H3	0.96306919981
H2	H3	0.04463244922
C1	H4	0.96678358027
H2	H4	0.044054363231
H3	H4	0.04405428833
C1	C5	0.97872663269
H2	C5	0.041641807837
H3	C5	0.041679841489
H4	C5	0.042025064344
C1	H6	0.044198132821
H2	H6	0.011760187943
H3	H6	0.0036990294686
H4	H6	0.0038671509385
C5	H6	0.95231984758
C1	C7	0.046282755366
H2	C7	0.0074034787909
H3	C7	0.0074201088701
H4	C7	0.01070963446
C5	C7	0.97875583771
H6	C7	0.044220957618
C1	H8	0.044211791902
H2	H8	0.0036990204158
H3	H8	0.011760171585
H4	H8	0.0038672042324
C5	H8	0.95219038502
H6	H8	0.043964373703
C7	H8	0.044212471313

C1	H9	0.010706929043
H2	H9	0.00081188893962
H3	H9	0.00081195903789
H4	H9	0.0023272657636
C5	H9	0.042015702455
H6	H9	0.0038670617269
C7	H9	0.96683321962
H8	H9	0.0038670533606
C1	C1	0.0074102759563
H2	C1	0.00052015775475
H3	C1	0.0060681230495
H4	C1	0.00081189364638
C5	C1	0.041685917194
H6	C1	0.0036991103427
C7	C1	0.96311553111
H8	C1	0.01176020523
H9	C1	0.044053954308
C1	H11	0.0074017040622
H2	H11	0.0060679909822
H3	H11	0.00052024525553
H4	H11	0.00081196489718
C5	H11	0.041636780928
H6	H11	0.011760185182
C7	H11	0.96307240601
H8	H11	0.0036989726702
H9	H11	0.044053859034
C1	H11	0.044632081626

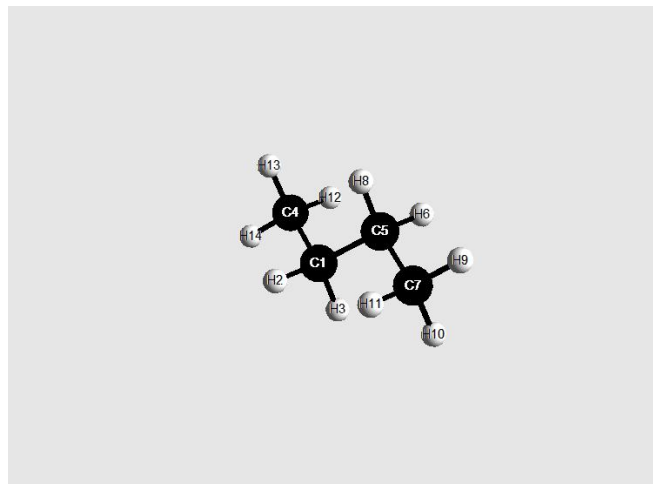
### CCSD

Atom A	Atom B	Delocalization index
C1	H2	0.82688113369
C1	H3	0.82687986306
H2	H3	0.034567833721
C1	H4	0.83143315133
H2	H4	0.034031544272
H3	H4	0.034030908823
C1	C5	0.84129840684
H2	C5	0.033015070828
H3	C5	0.033057500521
H4	C5	0.033197948339
C1	H6	0.035454006165
H2	H6	0.0093974215342
H3	H6	0.0032100442557
H4	H6	0.0033334787306
C5	H6	0.81703631628
C1	C7	0.040139759956
H2	C7	0.0070381882613
H3	C7	0.0070452621982



H4	C7	0.0083625646336
C5	C7	0.84126012076
H6	C7	0.035447486802
C1	H8	0.035436242522
H2	H8	0.0032099499409
H3	H8	0.0093973904652
H4	H8	0.0033335539144
C5	H8	0.81696119503
H6	H8	0.034101471869
C7	H8	0.035440459021
C1	H9	0.0083620702682
H2	H9	0.00074032173545
H3	H9	0.00074034671152
H4	H9	0.0021334703344
C5	H9	0.033188347037
H6	H9	0.0033334617802
C7	H9	0.83141307909
H8	H9	0.0033334515029
C1	C1	0.0070429609064
H2	C1	0.00055887148514
H3	C1	0.0069669083246
H4	C1	0.00074030370827
C5	C1	0.033056071838
H6	C1	0.0032100142601
C7	C1	0.8268632723
H8	C1	0.0093973996303
H9	C1	0.034030747735
C1	H11	0.0070408647949
H2	H11	0.0069668907282
H3	H11	0.00055895503653
H4	H11	0.00074034042816
C5	H11	0.033015001489
H6	H11	0.0093974214566
C7	H11	0.82688375414
H8	H11	0.0032100201005
H9	H11	0.034031370831
C1	H11	0.034567748078

## BUTANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	H2	0.94815544477
C1	H3	0.94804306252
H2	H3	0.044091742162
C1	C4	0.97899515716
H2	C4	0.043782104201
H3	C4	0.043782081641
C1	C5	0.96634514078
H2	C5	0.041931218859
H3	C5	0.041990749791
C4	C5	0.044326978833
C1	H6	0.041931525814
H2	H6	0.011402703981
H3	H6	0.0036814389059
C4	H6	0.0079645872427
C5	H6	0.94814968601
C1	C7	0.044331601866
H2	C7	0.0079651035898
H3	C7	0.0079842533121
C4	C7	0.0094133429015
C5	C7	0.97899824314
H6	C7	0.04378189073
C1	H8	0.04198968573
H2	H8	0.0036816284037
H3	H8	0.011402699275
C4	H8	0.0079835533953
C5	H8	0.94802845679
H6	H8	0.044092421633
C7	H8	0.043782127786
C1	H9	0.010375108983
H2	H9	0.00087523338133

H3	H9	0.0008752364712
C4	H9	0.001935747835
C5	H9	0.042117011336
H6	H9	0.0038760012496
C7	H9	0.96679741557
H8	H9	0.0038759762702
C1	C1	0.0071089169219
H2	C1	0.00055759119323
H3	C1	0.0067175246011
C4	C1	0.00080158584234
C5	C1	0.041530274268
H6	C1	0.0036702150818
C7	C1	0.96313652329
H8	C1	0.011582873905
H9	C1	0.044098783508
C1	H11	0.0071115600272
H2	H11	0.0067173915505
H3	H11	0.00055759850242
C4	H11	0.00080092238747
C5	H11	0.041461624018
H6	H11	0.011582866552
C7	H11	0.96305358244
H8	H11	0.0036702676969
H9	H11	0.044098281769
C1	H11	0.044603919277
C1	H12	0.041462054208
H2	H12	0.011582928388
H3	H12	0.0036702175609
C4	H12	0.96306662697
C5	H12	0.0071107155514
H6	H12	0.0067175492002
C7	H12	0.00080093353895
H8	H12	0.00055760797302
H9	H12	6.6037139016e-05
C1	H12	4.8577137224e-05
H11	H12	0.00037192707196
C1	H13	0.041529102852
H2	H13	0.0036703990955
H3	H13	0.011582907987
C4	H13	0.96313863952
C5	H13	0.0071074055141
H6	H13	0.0005575636899
C7	H13	0.00080155951667
H8	H13	0.0067172430338
H9	H13	6.6035618402e-05
C1	H13	0.0003719161429
H11	H13	4.8574179099e-05
H12	H13	0.04460584223

C1	H14	0.042117518056
H2	H14	0.0038760479896
H3	H14	0.003876012598
C4	H14	0.9668026587
C5	H14	0.010374778388
H6	H14	0.00087524085502
C7	H14	0.0019357464403
H8	H14	0.00087521848782
H9	H14	0.0004821137194
C1	H14	6.6035802945e-05
H11	H14	6.6035679942e-05
H12	H14	0.044099370222
H13	H14	0.044098799337

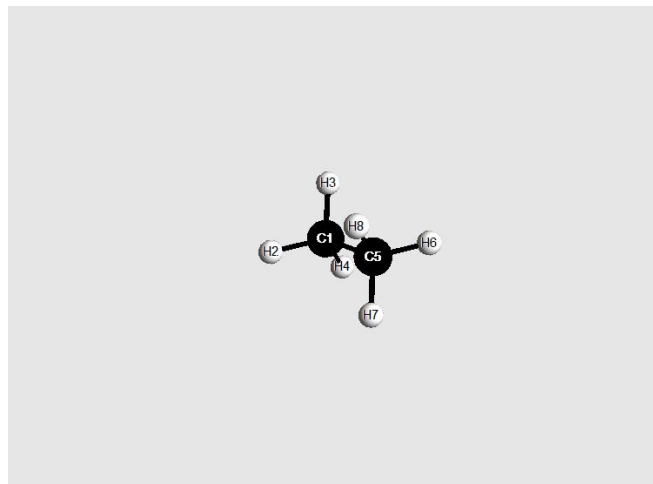
### CCSD

Atom A	Atom B	Delocalization index
C1	H2	0.81215849704
C1	H3	0.81217363219
H2	H3	0.034009732427
C1	C4	0.84152543781
H2	C4	0.034914021937
H3	C4	0.034910903635
C1	C5	0.82935212817
H2	C5	0.033402314491
H3	C5	0.033486153139
C4	C5	0.038105428107
C1	H6	0.033403815574
H2	H6	0.0091923594936
H3	H6	0.0032043141544
C4	H6	0.0075232266318
C5	H6	0.81213907064
C1	C7	0.038107919052
H2	C7	0.0075232530797
H3	C7	0.0075347640644
C4	C7	0.007314424399
C5	C7	0.84152580218
H6	C7	0.034913464831
C1	H8	0.033487502262
H2	H8	0.0032041364146
H3	H8	0.0091923703065
C4	H8	0.0075342234885
C5	H8	0.81217317863
H6	H8	0.034009106415
C7	H8	0.034910188444
C1	H9	0.0080647932154
H2	H9	0.00077322324501
H3	H9	0.00077331229319
C4	H9	0.0016667767474

C5	H9	0.033277813429
H6	H9	0.0033166585521
C7	H9	0.83132611061
H8	H9	0.0033166774611
C1	C1	0.0066230355032
H2	C1	0.00058375620495
H3	C1	0.0075848110892
C4	C1	0.00070501396105
C5	C1	0.032964194729
H6	C1	0.0031745486973
C7	C1	0.82693031649
H8	C1	0.0092041630899
H9	C1	0.034045192726
C1	H11	0.0066166510453
H2	H11	0.007584142927
H3	H11	0.00058381671297
C4	H11	0.00070463690707
C5	H11	0.032889258548
H6	H11	0.0092041704107
C7	H11	0.82691870456
H8	H11	0.0031746239346
H9	H11	0.034045307412
C1	H11	0.034490483298
C1	H12	0.032888869566
H2	H12	0.0092041678855
H3	H12	0.0031746097836
C4	H12	0.82691815417
C5	H12	0.0066153938242
H6	H12	0.0075846333639
C7	H12	0.0007046578026
H8	H12	0.00058380780321
H9	H12	7.5121904194e-05
C1	H12	5.5800397976e-05
H11	H12	0.0003803515941
C1	H13	0.032962388868
H2	H13	0.0031746902907
H3	H13	0.0092041699544
C4	H13	0.82692904138
C5	H13	0.0066225656538
H6	H13	0.00058377151907
C7	H13	0.00070497577553
H8	H13	0.0075843486289
H9	H13	7.5121365381e-05
C1	H13	0.00038035251904
H11	H13	5.579705285e-05
H12	H13	0.034490174377
C1	H14	0.033278060123
H2	H14	0.0033166639772

H3	H14	0.0033166971211
C4	H14	0.83132918448
C5	H14	0.0080645479773
H6	H14	0.00077329516289
C7	H14	0.0016667894742
H8	H14	0.00077327734267
H9	H14	0.00046944804861
C1	H14	7.5123907464e-05
H11	H14	7.5123977786e-05
H12	H14	0.03404525431
H13	H14	0.034045441615

## ETHANE



### HARTREE-FOCK

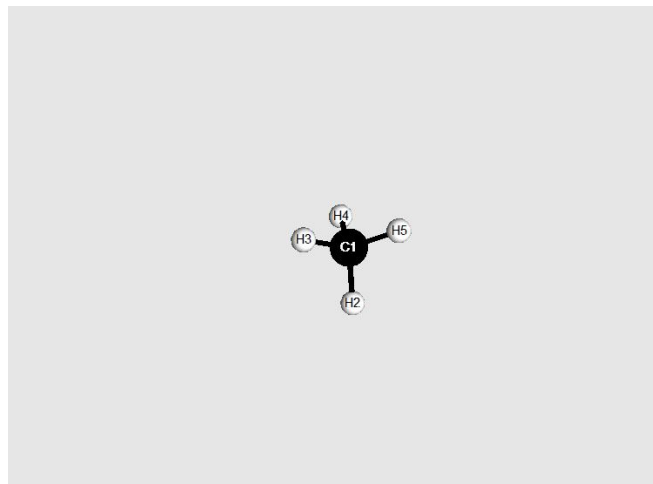
Atom A	Atom B	Delocalization index
C1	H2	0.967108982
C1	H3	0.96706373207
H2	H3	0.044529963053
C1	H4	0.96705909746
H2	H4	0.044529483749
H3	H4	0.044529476803
C1	C5	0.99215865008
H2	C5	0.043570326039
H3	C5	0.043566550693
H4	C5	0.04354153403
C1	H6	0.043569668413
H2	H6	0.012028820023
H3	H6	0.0036646197023
H4	H6	0.0036645792582
C5	H6	0.96710314263
C1	H7	0.043566229985
H2	H7	0.0036646339331
H3	H7	0.012028812514
H4	H7	0.0036645709624
C5	H7	0.96706347211
H6	H7	0.044528957538
C1	H8	0.04354181174
H2	H8	0.0036645891798
H3	H8	0.0036646382865
H4	H8	0.012028826208
C5	H8	0.96706271957
H6	H8	0.044529282204
H7	H8	0.044529424004

## CCSD

Atom A	Atom B	Delocalization index
C1	H2	0.83164503207
C1	H3	0.8316976086
H2	H3	0.034665310739
C1	H4	0.83167896479
H2	H4	0.034665045721
H3	H4	0.03466505042
C1	C5	0.85419411785
H2	C5	0.034751011055
H3	C5	0.034757264099
H4	C5	0.034749135734
C1	H6	0.03475113226
H2	H6	0.0095474343391
H3	H6	0.0031755061834
H4	H6	0.0031754892058
C5	H6	0.83164176327
C1	H7	0.034757292276
H2	H7	0.0031755402336
H3	H7	0.0095474018403
H4	H7	0.00317548122
C5	H7	0.83169855829
H6	H7	0.034665028145
C1	H8	0.03474938745
H2	H8	0.003175441917
H3	H8	0.0031753981452
H4	H8	0.0095474141558
C5	H8	0.83168105973
H6	H8	0.034665246001
H7	H8	0.034665224294



## METHANE



### HARTREE-FOCK

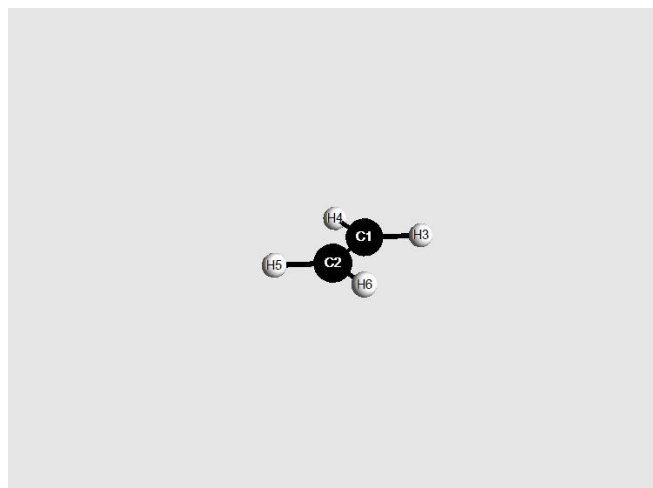
Atom A	Atom B	Delocalization index
C1	H2	0.98182690831
C1	H3	0.98182826084
H2	H3	0.044325072993
C1	H4	0.98182465674
H2	H4	0.044325690147
H3	H4	0.044329124455
C1	H5	0.98182254623
H2	H5	0.044326511579
H3	H5	0.044328169017
H4	H5	0.044327994963

### CCSD

Atom A	Atom B	Delocalization index
C1	H2	0.84645544956
C1	H3	0.84648982576
H2	H3	0.034455352181
C1	H4	0.84648623937
H2	H4	0.034457030782
H3	H4	0.034486193421
C1	H5	0.846487614
H2	H5	0.034458731313
H3	H5	0.034482410658
H4	H5	0.034482581631

# ALKENES

## ETHYLENE



### HARTREE-FOCK

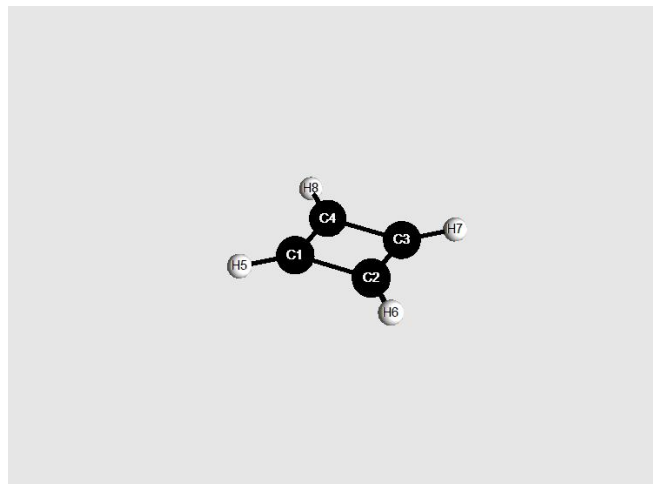
Atom A	Atom B	Delocalization index
C1	C2	1.8821280045
C1	H3	0.98404062747
C2	H3	0.068315013865
C1	H4	0.98407121483
C2	H4	0.068308777675
H3	H4	0.037524578345
C1	H5	0.068314859998
C2	H5	0.98403998682
H3	H5	0.012877523587
H4	H5	0.0076595304555
C1	H6	0.068308703514
C2	H6	0.98407118365
H3	H6	0.0076595330212
H4	H6	0.01287755812
H5	H6	0.037524547534

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.4937280008
C1	H3	0.84937633633
C2	H3	0.048589058275
C1	H4	0.8493825996
C2	H4	0.048586586178
H3	H4	0.029534214674
C1	H5	0.048589119239
C2	H5	0.849377102
H3	H5	0.010476501835
H4	H5	0.0059876070246

C1	H6	0.048586579429
C2	H6	0.84938256659
H3	H6	0.0059876026129
H4	H6	0.010476517115
H5	H6	0.029534242996

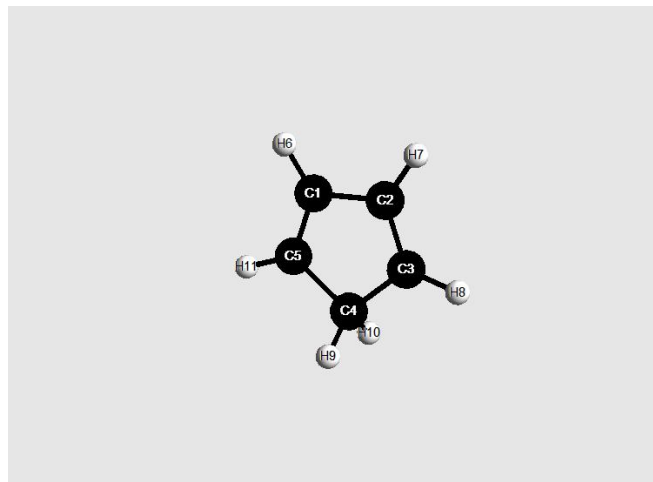
## CYCLOBUTADIENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.97751134223
C1	C3	0.14083699262
C2	C3	1.8501542947
C1	C4	1.8501540062
C2	C4	0.14062672489
C3	C4	0.97757550471
C1	H5	0.98281139425
C2	H5	0.035953575209
C3	H5	0.014774977417
C4	H5	0.063127510888
C1	H6	0.035954015423
C2	H6	0.98283509659
C3	H6	0.063126832461
C4	H6	0.014772991234
H5	H6	0.0011647337596
C1	H7	0.014779518214
C2	H7	0.063127836692
C3	H7	0.98281090622
C4	H7	0.035948911979
H5	H7	0.0048580011031
H6	H7	0.0034878651297
C1	H8	0.063135324794
C2	H8	0.014776994683
C3	H8	0.035948822337
C4	H8	0.98283551934
H5	H8	0.0034887175165
H6	H8	0.0048580111389
H7	H8	0.0011640893452

## CYCLOPENTADIENE

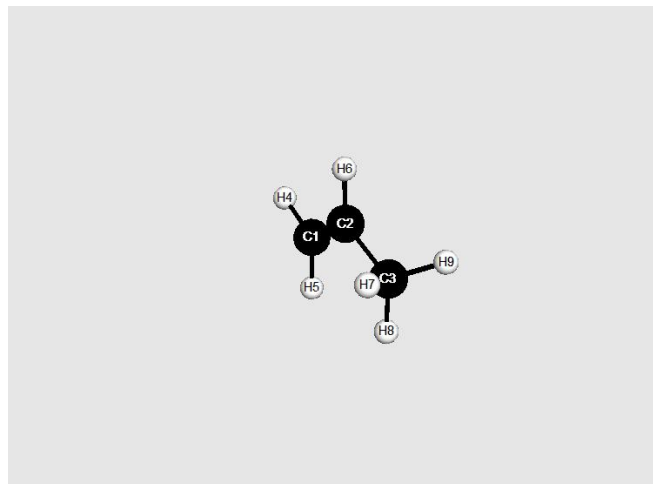


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.0795099051
C1	C3	0.082305230315
C2	C3	1.7398921709
C1	C4	0.072694177007
C2	C4	0.072702786954
C3	C4	1.0030595903
C1	C5	1.7398416853
C2	C5	0.082331596798
C3	C5	0.11913281346
C4	C5	1.0031119417
C1	H6	0.98318037784
C2	H6	0.036339293481
C3	H6	0.007290531713
C4	H6	0.010803442596
C5	H6	0.061312998322
C1	H7	0.036328590706
C2	H7	0.98325547078
C3	H7	0.061301134624
C4	H7	0.010803145451
C5	H7	0.0072909924409
H6	H7	0.0019435449741
C1	H8	0.010838622027
C2	H8	0.060805470595
C3	H8	0.98456960207
C4	H8	0.03530692687
C5	H8	0.013371631082
H6	H8	0.0015904836835
H7	H8	0.0044047952585
C1	H9	0.01861369551
C2	H9	0.018613557086

C3	H9	0.047461210798
C4	H9	0.93985403632
C5	H9	0.047465721353
H6	H9	0.0016831561839
H7	H9	0.0016831623049
H8	H9	0.0016735796844
C1	C1	0.01855223117
C2	C1	0.018554052902
C3	C1	0.047365058501
C4	C1	0.94010885351
C5	C1	0.047362583117
H6	C1	0.0016833457443
H7	C1	0.0016833353319
H8	C1	0.0016724346873
H9	C1	0.0389767512
C1	H11	0.060798400745
C2	H11	0.010840632854
C3	H11	0.013370466456
C4	H11	0.035310170814
C5	H11	0.98460242453
H6	H11	0.0044048439854
H7	H11	0.001590478604
H8	H11	0.0018504020716
H9	H11	0.0016736084397
C1	H11	0.001672435363

## ALLYL



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.8392225423
C1	C3	0.064183776142
C2	C3	1.0172231777
C1	H4	0.98716878016
C2	H4	0.069046684063
C3	H4	0.011147252784
C1	H5	0.98169828117
C2	H5	0.067997948849
C3	H5	0.011074816064
H4	H5	0.037850976034
C1	H6	0.068282243735
C2	H6	0.9730225872
C3	H6	0.038584001503
H4	H6	0.0080269734012
H5	H6	0.013068400912
C1	H7	0.019262772471
C2	H7	0.047294631089
C3	H7	0.95975598556
H4	H7	0.0017736212098
H5	H7	0.0012083550444
H6	H7	0.0027336017972
C1	H8	0.012027306392
C2	H8	0.043783347419
C3	H8	0.95991936884
H4	H8	0.00097285494801
H5	H8	0.008297844831
H6	H8	0.010369803879
H7	H8	0.04160285443
C1	H9	0.019260824472
C2	H9	0.047297332676

C3	H9	0.95970894607
H4	H9	0.001773621715
H5	H9	0.0012083478183
H6	H9	0.0027343504521
H7	H9	0.043112379467
H8	H9	0.04160214995

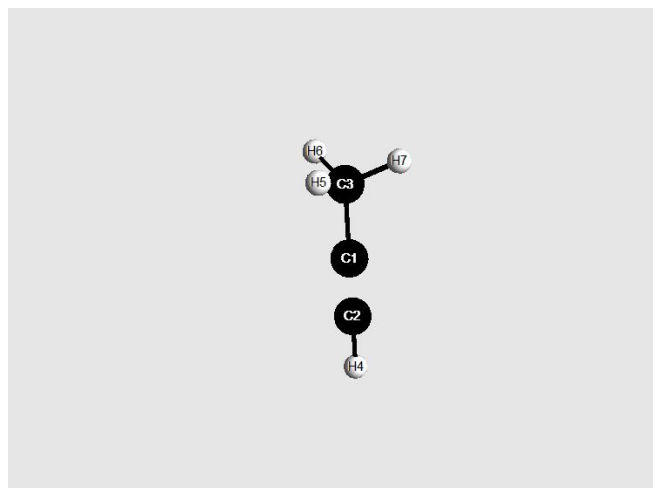
#### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.4634904463
C1	C3	0.049398241095
C2	C3	0.87987476281
C1	H4	0.85262303971
C2	H4	0.04843744503
C3	H4	0.0088137178803
C1	H5	0.84633517292
C2	H5	0.047466523516
C3	H5	0.0094051928071
H4	H5	0.02935855622
C1	H6	0.049475823555
C2	H6	0.83787497103
C3	H6	0.030979391188
H4	H6	0.0062519034239
H5	H6	0.010641956079
C1	H7	0.013493122995
C2	H7	0.036914929561
C3	H7	0.82634253792
H4	H7	0.0014939386332
H5	H7	0.000961042005
H6	H7	0.0023436884049
C1	H8	0.011237141684
C2	H8	0.034083584262
C3	H8	0.82449331873
H4	H8	0.00088546482267
H5	H8	0.009831558393
H6	H8	0.0084202806428
H7	H8	0.032457702441
C1	H9	0.013492292165
C2	H9	0.03691541391
C3	H9	0.82631787379
H4	H9	0.0014939486028
H5	H9	0.00096105959495
H6	H9	0.0023438692121
H7	H9	0.033861939998
H8	H9	0.032457488113



# ALKYNES

## PROPYNE



### HARTREE-FOCK

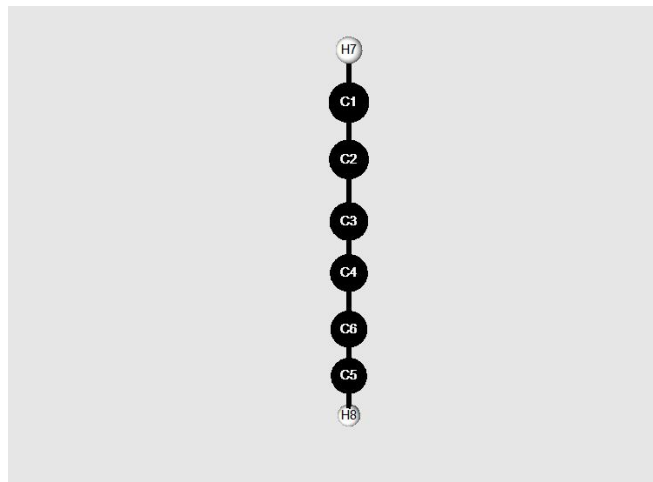
Atom A	Atom B	Delocalization index
C1	C2	1.8005308309
C1	C3	1.0344881156
C2	C3	0.058245517946
C1	H4	0.062079116968
C2	H4	0.97138365057
C3	H4	0.0028193899193
C1	H5	0.05147835457
C2	H5	0.019726591292
C3	H5	0.95064835371
H4	H5	0.00079034237851
C1	H6	0.051460317748
C2	H6	0.019727174434
C3	H6	0.95070155423
H4	H6	0.00079030180535
H5	H6	0.037688161536
C1	H7	0.051452286249
C2	H7	0.019729524261
C3	H7	0.95071349393
H4	H7	0.00079021877812
H5	H7	0.037686963614
H6	H7	0.03768487073

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	2.1500479679
C1	C3	0.9229342433
C2	C3	0.048367672676
C1	H4	0.055114296698

C2	H4	0.85530362622
C3	H4	0.0026118368436
C1	H5	0.040745551366
C2	H5	0.015126674809
C3	H5	0.81915134044
H4	H5	0.00066013018807
C1	H6	0.040743798952
C2	H6	0.015129568654
C3	H6	0.81926167262
H4	H6	0.00065995908738
H5	H6	0.030151353044
C1	H7	0.040745798051
C2	H7	0.015126622003
C3	H7	0.8192426493
H4	H7	0.00066015297216
H5	H7	0.030151938759
H6	H7	0.030151378643

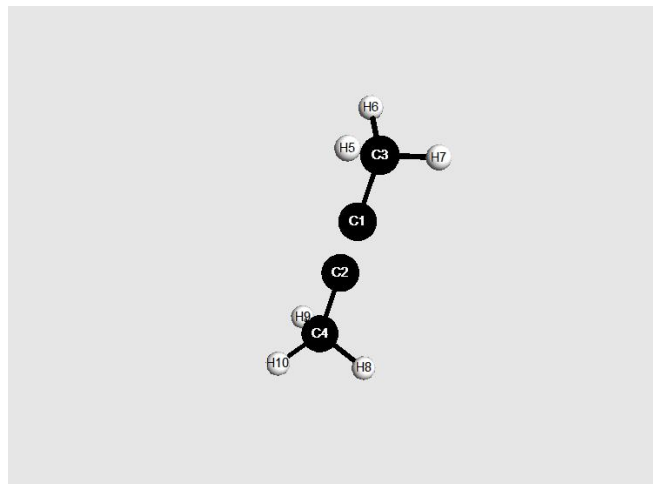
### 1,3,5-HEXATRIYNE-HF



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	2.072579661
C1	C3	0.059459840161
C2	C3	1.0872262608
C1	C4	0.073388299956
C2	C4	0.055674871574
C3	C4	1.97562699
C1	C5	0.015086660206
C2	C5	0.0048421805753
C3	C5	0.073388139875
C4	C5	0.059459813881
C1	C6	0.0048421875065
C2	C6	0.0039541214528
C3	C6	0.055674843132
C4	C6	1.0872257624
C5	C6	2.0725801795
C1	H7	0.84806330431
C2	H7	0.04841973406
C3	H7	0.0026230747886
C4	H7	0.0030506863172
C5	H7	0.00073020892202
C6	H7	0.00022733601604
C1	H8	0.00073020960003
C2	H8	0.00022733603983
C3	H8	0.0030506850819
C4	H8	0.0026230758411
C5	H8	0.84806385764
C6	H8	0.04841978492
H7	H8	4.1918439459e-05

## 2-BUTYNE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.757006665
C1	C3	1.0370527861
C2	C3	0.05815826813
C1	C4	0.058185802408
C2	C4	1.0371491288
C3	C4	0.00277234493
C1	H5	0.050635030442
C2	H5	0.018798661691
C3	H5	0.95218195522
C4	H5	0.00077038078043
C1	H6	0.05063646934
C2	H6	0.018798030759
C3	H6	0.9522992298
C4	H6	0.00077029174017
H5	H6	0.03869677926
C1	H7	0.050638615183
C2	H7	0.018797307694
C3	H7	0.95227453286
C4	H7	0.00077024260632
H5	H7	0.038697903561
H6	H7	0.038696752986
C1	H8	0.018797821553
C2	H8	0.050632861061
C3	H8	0.00076996661017
C4	H8	0.95227569672
H5	H8	0.00020442638345
H6	H8	0.00020537068783
H7	H8	0.00081896202829
C1	H9	0.018796095657
C2	H9	0.050633396076

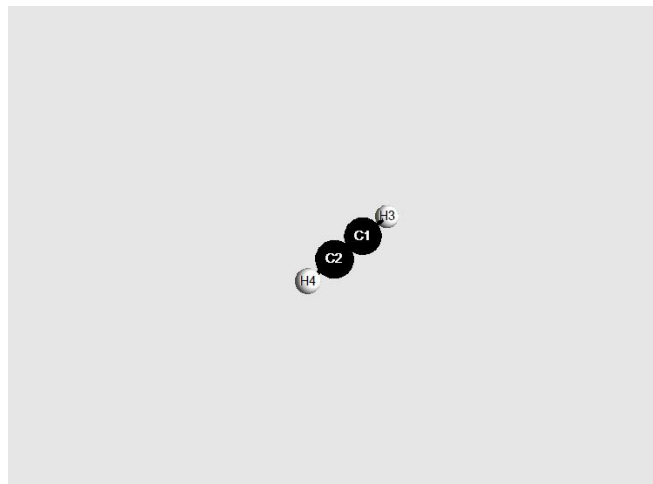
C3	H9	0.00077012610386
C4	H9	0.95229249685
H5	H9	0.00020531665737
H6	H9	0.00081889408639
H7	H9	0.00020434005587
H8	H9	0.038696706833
C1	C1	0.018796927887
C2	C1	0.050637967777
C3	C1	0.00076923371623
C4	C1	0.95232111323
H5	C1	0.00081897463505
H6	C1	0.00020439132796
H7	C1	0.00020531557437
H8	C1	0.038698435866
H9	C1	0.038697149753

### CCSD

Atom A	Atom B	Delocalization index
C1	H2	0.82004877368
C1	H3	0.82002366237
H2	H3	0.030850924244
C1	H4	0.8200756367
H2	H4	0.030850976594
H3	H4	0.030850702191
C1	C5	0.0025058927313
H2	C5	0.00064295644139
H3	C5	0.00064281000648
H4	C5	0.00064290653294
C1	H6	0.00064289203163
H2	H6	0.00022425410225
H3	H6	0.00022424759327
H4	H6	0.00056977839976
C5	H6	0.82008695185
C1	H7	0.00064276943989
H2	H7	0.00022424775548
H3	H7	0.00056990055479
H4	H7	0.00022420746115
C5	H7	0.82003251263
H6	H7	0.030849935102
C1	H8	0.00064290602696
H2	H8	0.00056982542706
H3	H8	0.00022420840973
H4	H8	0.00022426710177
C5	H8	0.82005273344
H6	H8	0.030852165561
H7	H8	0.03085210204
C1	C9	0.92209751322
H2	C9	0.040134714107

H3	C9	0.040134823856
H4	C9	0.040135102545
C5	C9	0.050425168735
H6	C9	0.014839881954
H7	C9	0.014840502456
H8	C9	0.014839847211
C1	C1	0.050425983339
H2	C1	0.014841715462
H3	C1	0.014842083144
H4	C1	0.014840954353
C5	C1	0.92207666521
H6	C1	0.040134495459
H7	C1	0.040133668058
H8	C1	0.040134594003
C9	C1	2.117268205

## ACETYLENE



### HARTREE-FOCK

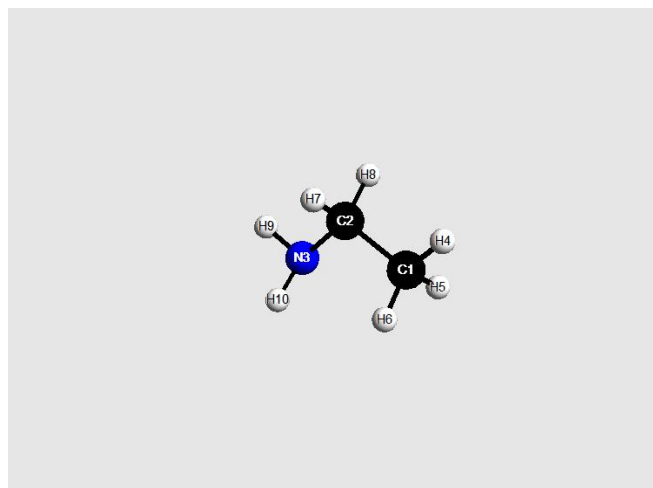
Atom A	Atom B	Delocalization index
C1	C2	1.8248421587
C1	H3	0.96355743756
C2	H3	0.060236086441
C1	H4	0.060236099527
C2	H4	0.96355761987
H3	H4	0.0027444267078

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	2.1969580828
C1	H3	0.85191036328
C2	H3	0.051778619394
C1	H4	0.051778661486
C2	H4	0.85191082989
H3	H4	0.0027405223841

# AMINES

## ETHYLAMINE



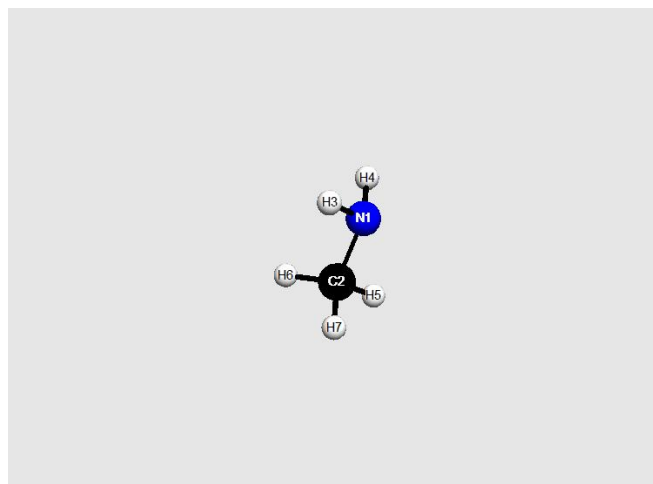
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.95993117312
C1	N3	0.074953378086
C2	N3	0.95258974339
C1	H4	0.96703788567
C2	H4	0.041867113558
N3	H4	0.012983158722
C1	H5	0.96043258963
C2	H5	0.039733102561
N3	H5	0.015326052331
H4	H5	0.042366729299
C1	H6	0.96318384926
C2	H6	0.041958190721
N3	H6	0.010536072287
H4	H6	0.044645446052
H5	H6	0.043694762341
C1	H7	0.044855661511
C2	H7	0.93128245875
N3	H7	0.078248994519
H4	H7	0.0041440518521
H5	H7	0.011589693961
H6	H7	0.0039228283999
C1	H8	0.042156089312
C2	H8	0.93054739323
N3	H8	0.064774415679
H4	H8	0.0037276645367
H5	H8	0.0039451914488
H6	H8	0.011527507159
H7	H8	0.042967020707



C1	H9	0.0087905844579
C2	H9	0.021282292378
N3	H9	0.88916749049
H4	H9	0.002033989813
H5	H9	0.00050484861554
H6	H9	0.00059610408806
H7	H9	0.0020523887265
H8	H9	0.0022228548955
C1	C1	0.0045233430488
C2	C1	0.021685316808
N3	C1	0.88876532203
H4	C1	0.00052039238096
H5	C1	0.0003353020198
H6	C1	0.0036834474999
H7	C1	0.0023877381859
H8	C1	0.0099076949235
H9	C1	0.018578902262

## METHYLAMINE



### HARTREE-FOCK

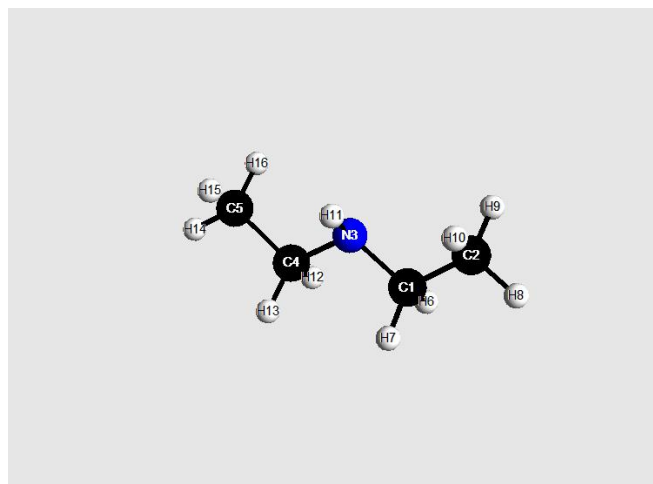
Atom A	Atom B	Delocalization index
N1	C2	0.9788652564
N1	H3	0.88819682804
C2	H3	0.022326851164
N1	H4	0.88816237498
C2	H4	0.022324081816
H3	H4	0.018708222848
N1	H5	0.064018211314
C2	H5	0.94449429281
H3	H5	0.0097165183431
H4	H5	0.0020796994784
N1	H6	0.077755205349
C2	H6	0.94540015558
H3	H6	0.0022471881548
H4	H6	0.0022471879621
H5	H6	0.043582857975
N1	H7	0.064014166012
C2	H7	0.94466584777
H3	H7	0.0020796910554
H4	H7	0.0097165452828
H5	H7	0.041906297365
H6	H7	0.043583397503

### CCSD

Atom A	Atom B	Delocalization index
N1	C2	0.86931435577
N1	H3	0.78118942041
C2	H3	0.021574321261
N1	H4	0.78126642182
C2	H4	0.021571632877
H3	H4	0.018231331996

N1	H5	0.048372447487
C2	H5	0.81552339819
H3	H5	0.0082053881086
H4	H5	0.0020191026907
N1	H6	0.059090276117
C2	H6	0.81582819486
H3	H6	0.0023618519954
H4	H6	0.0023618277822
H5	H6	0.033824252549
N1	H7	0.048360032041
C2	H7	0.81564764347
H3	H7	0.0020191320457
H4	H7	0.0082053843463
H5	H7	0.032784205008
H6	H7	0.033824385474

## DIETHYLAMINE



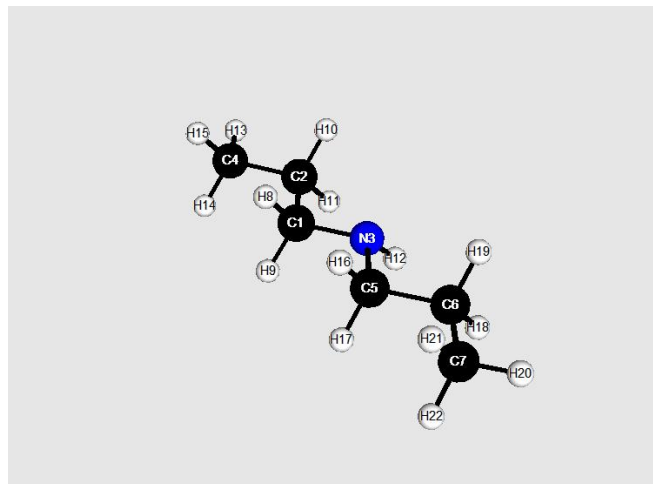
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.95981063294
C1	N3	0.94489981345
C2	N3	0.072319418633
C1	C4	0.029199763532
C2	C4	0.0084853010762
N3	C4	0.94521593364
C1	C5	0.0084828452002
C2	C5	0.0015276184404
N3	C5	0.072327802209
C4	C5	0.95986725218
C1	H6	0.92440454535
C2	H6	0.041472115327
N3	H6	0.062528244071
C4	H6	0.0074649530409
C5	H6	0.00091597031831
C1	H7	0.92223512129
C2	H7	0.043935569706
N3	H7	0.075880344772
C4	H7	0.0078926571226
C5	H7	0.001090711784
H6	H7	0.043175136612
C1	H8	0.041794050236
C2	H8	0.96688332614
N3	H8	0.012464148436
C4	H8	0.0017809745238
C5	H8	0.00034837600414
H6	H8	0.0037710243723
H7	H8	0.0041076531562
C1	H9	0.039603562074
C2	H9	0.96090823857

N3	H9	0.014665782615
C4	H9	0.00061299011266
C5	H9	7.7305057993e-05
H6	H9	0.0038603800236
H7	H9	0.011364408845
H8	H9	0.042439828474
C1	C1	0.041749889541
C2	C1	0.9631878388
N3	C1	0.010129537442
C4	C1	0.00066947991331
C5	C1	6.3479688272e-05
H6	C1	0.011235292179
H7	C1	0.0038680288485
H8	C1	0.04459348701
H9	C1	0.043751879425
C1	H11	0.020991577114
C2	H11	0.0059102455102
N3	H11	0.87564557738
C4	H11	0.020965821764
C5	H11	0.0059118133836
H6	H11	0.0094228194359
H7	H11	0.0020271806781
H8	H11	0.00064741824023
H9	H11	0.00038360552089
C1	H11	0.0048148786152
C1	H12	0.0074614493533
C2	H12	0.00091590761707
N3	H12	0.062530094381
C4	H12	0.92440203799
C5	H12	0.04147204143
H6	H12	0.0091238225433
H7	H12	0.00073837344647
H8	H12	5.9004921064e-05
H9	H12	5.8082035207e-05
C1	H12	0.00044651999831
H11	H12	0.0094228058501
C1	H13	0.0078718896099
C2	H13	0.0010902884143
N3	H13	0.07586721912
C4	H13	0.9223772557
C5	H13	0.043894756761
H6	H13	0.00073842211679
H7	H13	0.010052224569
H8	H13	0.0001006627783
H9	H13	0.00051204661827
C1	H13	6.6164160872e-05
H11	H13	0.0020273039063
H12	H13	0.04317564478

C1	H14	0.0017808062146
C2	H14	0.00034840161857
N3	H14	0.012462694379
C4	H14	0.041809727454
C5	H14	0.96681548883
H6	H14	5.9005005449e-05
H7	H14	0.00010065891004
H8	H14	0.00013986335907
H9	H14	1.6064844199e-05
C1	H14	1.7759844134e-05
H11	H14	0.00064738545334
H12	H14	0.0037710761539
H13	H14	0.0041076662341
C1	H15	0.00066929801312
C2	H15	6.3472224503e-05
N3	H15	0.010123821191
C4	H15	0.041727366966
C5	H15	0.96311456124
H6	H15	0.0004465138681
H7	H15	6.6158111521e-05
H8	H15	1.775961567e-05
H9	H15	5.2241839545e-06
C1	H15	2.1270078643e-05
H11	H15	0.0048148551141
H12	H15	0.011235299906
H13	H15	0.0038678389808
H14	H15	0.04459384262
C1	H16	0.00061194142047
C2	H16	7.7286315152e-05
N3	H16	0.014664433891
C4	H16	0.039709773693
C5	H16	0.96093832199
H6	H16	5.8078266664e-05
H7	H16	0.00051203155067
H8	H16	1.6064574736e-05
H9	H16	2.5568157992e-05
C1	H16	5.2243584329e-06
H11	H16	0.0003835995622
H12	H16	0.0038602216363
H13	H16	0.011364429469
H14	H16	0.042439720959
H15	H16	0.043751849145

## DIPROPYLAMINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.94764690535
C1	N3	0.94451006105
C2	N3	0.069124009458
C1	C4	0.043458984226
C2	C4	0.97835613498
N3	C4	0.011006379113
C1	C5	0.029265766602
C2	C5	0.0082453221557
N3	C5	0.94460912186
C4	C5	0.0014810240004
C1	C6	0.0082453010009
C2	C6	0.0014218821048
N3	C6	0.069162630177
C4	C6	0.00027090617505
C5	C6	0.9477759187
C1	C7	0.0014806480285
C2	C7	0.00027080059496
N3	C7	0.011003877665
C4	C7	9.1655599979e-05
C5	C7	0.043470258067
C6	C7	0.9784332806
C1	H8	0.9206527986
C2	H8	0.039244316143
N3	H8	0.062002018959
C4	H8	0.0076126315329
C5	H8	0.00756387589
C6	H8	0.00089508468684
C7	H8	5.6034230962e-05
C1	H9	0.91806678689
C2	H9	0.041451910821

N3	H9	0.074868577027
C4	H9	0.0084710166837
C5	H9	0.0077766887652
C6	H9	0.0010338269926
C7	H9	8.5468048987e-05
H8	H9	0.043211909369
C1	C1	0.039939515906
C2	C1	0.94695326826
N3	C1	0.016034850783
C4	C1	0.041959443014
C5	C1	0.0006403529984
C6	C1	6.228499249e-05
C7	C1	1.2653252113e-05
H8	C1	0.003842285874
H9	C1	0.010903776039
C1	H11	0.041882653918
C2	H11	0.94840678399
N3	H11	0.011056178801
C4	H11	0.044106388669
C5	H11	0.00071796884244
C6	H11	5.3140347002e-05
C7	H11	1.658662429e-05
H8	H11	0.010806837661
H9	H11	0.0037743485659
C1	H11	0.043336912004
C1	H12	0.020833744854
C2	H12	0.005651772594
N3	H12	0.87522044932
C4	H12	0.00061616376894
C5	H12	0.020905097118
C6	H12	0.0056604484563
C7	H12	0.00061599151179
H8	H12	0.0093174933651
H9	H12	0.0020220897989
C1	H12	0.00041081912998
H11	H12	0.0053371341039
C1	H13	0.009986260547
C2	H13	0.04242552553
N3	H13	0.0019940759306
C4	H13	0.96661073821
C5	H13	0.00033399512214
C6	H13	0.00010652573187
C7	H13	2.88145434e-05
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H9	H13	0.00099741821021
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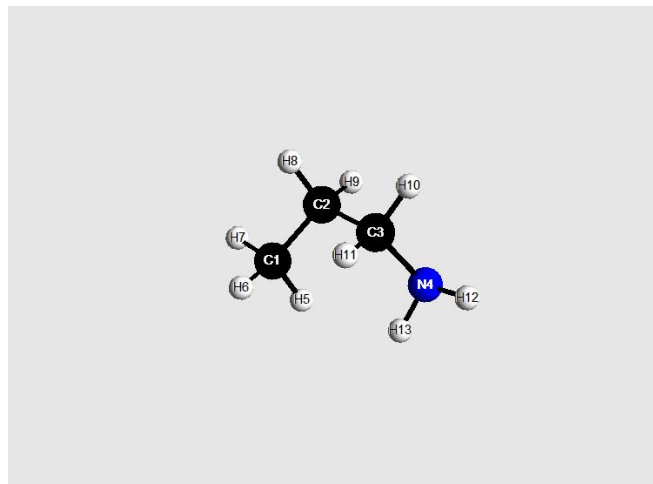
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C1	H14	0.011325683005
H11	H14	0.0037092960659
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C1	H15	0.0068252101035
C2	H15	0.041664475978
N3	H15	0.00098571162018
C4	H15	0.96324950183
C5	H15	5.4323715668e-05
C6	H15	1.3689384626e-05
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C1	H15	0.0035505973931
H11	H15	0.011636905935
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H14	H15	0.044878238966
C1	H16	0.0075549437269
C2	H16	0.00089449726104
N3	H16	0.06199181359
C4	H16	5.6070958497e-05
C5	H16	0.920445094
C6	H16	0.039314473627
C7	H16	0.0076058411528
H8	H16	0.0093022041327
H9	H16	0.00073348574939
C1	H16	5.9367282736e-05
H11	H16	0.0004611982846
H12	H16	0.0093174398535
H13	H16	1.2350959124e-05
H14	H16	7.5704702198e-06
H15	H16	2.340665326e-05
C1	H17	0.0077683615729
C2	H17	0.0010330848192
N3	H17	0.074868208734
C4	H17	8.5468314343e-05
C5	H17	0.91805239946
C6	H17	0.041481833637

C7	H17	0.0084732965001
H8	H17	0.00073349930858
H9	H17	0.0098744016154
C1	H17	0.00053179684066
H11	H17	6.8410723005e-05
H12	H17	0.0020221393582
H13	H17	1.3085337733e-05
H14	H17	4.7015793574e-05
H15	H17	7.0338049435e-06
H16	H17	0.043212444581
C1	H18	0.00071771087271
C2	H18	5.3052378944e-05
N3	H18	0.011048357364
C4	H18	1.659273621e-05
C5	H18	0.042009921157
C6	H18	0.94823144515
C7	H18	0.044093435577
H8	H18	0.00046117706912
H9	H18	6.8397570836e-05
C1	H18	5.4003147687e-06
H11	H18	2.0681948484e-05
H12	H18	0.0053370081828
H13	H18	3.0847741522e-06
H14	H18	1.4163290195e-06
H15	H18	3.3306334935e-06
H16	H18	0.010806682432
H17	H18	0.0037742216499
C1	H19	0.00064002111115
C2	H19	6.2192149038e-05
N3	H19	0.016033909455
C4	H19	1.2651783737e-05
C5	H19	0.039891000508
C6	H19	0.94698529963
C7	H19	0.041952863603
H8	H19	5.9367633512e-05
H9	H19	0.00053179761841
C1	H19	2.591044035e-05
H11	H19	5.4009047349e-06
H12	H19	0.00041085058051
H13	H19	2.6427942217e-06
H14	H19	5.2492346865e-06
H15	H19	1.05507567e-06
H16	H19	0.0038421217912
H17	H19	0.010903752394
H18	H19	0.043336233826
C1	C2	0.00033392590787
C2	C2	0.00010651242854
N3	C2	0.0019940384521

C4	C2	2.8816524138e-05
C5	C2	0.0099871407807
C6	C2	0.042446466863
C7	C2	0.96656208692
H8	C2	1.2351626171e-05
H9	C2	1.3084969248e-05
C1	C2	2.6427098203e-06
H11	C2	3.085379411e-06
H12	C2	2.544655713e-05
H13	C2	1.0090718424e-05
H14	C2	1.0622468494e-06
H15	C2	9.4806116882e-07
H16	C2	0.0008467462228
H17	C2	0.00099739675426
H18	C2	0.003951714013
H19	C2	0.003774197737
C1	H21	5.4238368806e-05
C2	H21	1.3680389146e-05
N3	H21	0.00098528578959
C4	H21	4.040752776e-06
C5	H21	0.0068332902054
C6	H21	0.041727064904
C7	H21	0.96323253892
H8	H21	2.3405722337e-05
H9	H21	7.0327863354e-06
C1	H21	1.0554190961e-06
H11	H21	3.3310426527e-06
H12	H21	0.00028499975552
H13	H21	9.4828313234e-07
H14	H21	2.4819322884e-07
H15	H21	4.820795376e-07
H16	H21	0.0064373290093
H17	H21	0.00062976362592
H18	H21	0.011636811817
H19	H21	0.0035505421194
C2	H21	0.044331722279
C1	H22	7.2527545753e-05
C2	H22	1.9741480781e-05
N3	H22	0.0016240916485
C4	H22	5.1817287328e-06
C5	H22	0.0067966866628
C6	H22	0.04174621219
C7	H22	0.96336838623
H8	H22	7.5708054163e-06
H9	H22	4.7016338088e-05
C1	H22	5.24912094e-06
H11	H22	1.4165137492e-06
H12	H22	4.4659247858e-05

H13	H22	1.0620860707e-06
H14	H22	1.1489092597e-06
H15	H22	2.4829521098e-07
H16	H22	0.00057165833671
H17	H22	0.0074824405052
H18	H22	0.003709304189
H19	H22	0.011325660569
C2	H22	0.044413182901
H21	H22	0.044878411688

## PROPYLAMINE



## HARTREE-FOCK

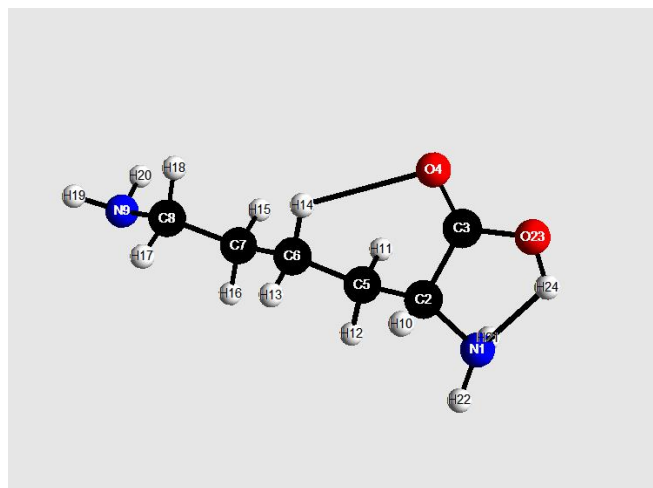
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C1	C2	0.97652467925
C1	C3	0.041245474113
C2	C3	0.94815322933
C1	N4	0.013654144283
C2	N4	0.068385161031
C3	N4	0.95106585831
C1	H5	0.96014492374
C2	H5	0.040610158243
C3	H5	0.0030882579996
N4	H5	0.014110428552
C1	H6	0.96330578107
C2	H6	0.041998759807
C3	H6	0.0072044171823
N4	H6	0.0016003576096
H5	H6	0.044841973859
C1	H7	0.96572494323
C2	H7	0.042196745825
C3	H7	0.010152845416
N4	H7	0.0016373471442
H5	H7	0.044177573971
H6	H7	0.044530399967
C1	H8	0.0445218324
C2	H8	0.95207905068
C3	H8	0.043566695619
N4	H8	0.011980430317
H5	H8	0.011524376013
H6	H8	0.0034401357579
H7	H8	0.0044896650473
C1	H9	0.042973030712
C2	H9	0.9469920518

C3	H9	0.040300529129
N4	H9	0.015713452264
H5	H9	0.0037365701206
H6	H9	0.011542547526
H7	H9	0.0034537330756
H8	H9	0.042236644631
C1	C1	0.0099036063163
C2	C1	0.04142016875
C3	C1	0.93044023586
N4	C1	0.0649028815
H5	C1	0.00044642873517
H6	C1	0.00075170630131
H7	C1	0.0018080124077
H8	C1	0.0049455371217
H9	C1	0.0039348320716
C1	H11	0.0076369476718
C2	H11	0.043082161865
C3	H11	0.9272696825
N4	H11	0.078329240361
H5	H11	0.0004173701265
H6	H11	0.0066678155343
H7	H11	0.00079797726724
H8	H11	0.0040127024012
H9	H11	0.011257096816
C1	H11	0.042477948405
C1	H12	0.00085190626303
C2	H12	0.0082638215863
C3	H12	0.021421716227
N4	H12	0.88823529004
H5	H12	0.00094682770472
H6	H12	6.091132084e-05
H7	H12	0.00010505722649
H8	H12	0.0016234074149
H9	H12	0.00045970874844
C1	H12	0.0029167624426
H11	H12	0.0017295835623
C1	H13	0.0059920558673
C2	H13	0.0018814081168
C3	H13	0.0211806628
N4	H13	0.8832255114
H5	H13	0.0075380256827
H6	H13	0.00060322560507
H7	H13	0.0010134343127
H8	H13	0.00028933348391
H9	H13	0.00027676963617
C1	H13	0.0094548304607
H11	H13	0.0027248352875
H12	H13	0.018217967893



# AMINOACIDS

## LYSINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.94118393624
N1	C3	0.057100116566
C2	C3	0.85509991425
N1	O4	0.014227833559
C2	O4	0.10040425676
C3	O4	1.1096808632
N1	C5	0.071738457116
C2	C5	0.93767363067
C3	C5	0.032789284475
O4	C5	0.024399363905
N1	C6	0.011420632134
C2	C6	0.03825966362
C3	C6	0.0018180982958
O4	C6	0.018410984724
C5	C6	0.96336932591
N1	C7	0.0018064505585
C2	C7	0.0085529424635
C3	C7	0.00031743954803
O4	C7	0.0015197566926
C5	C7	0.044610563727
C6	C7	0.96709163154
N1	C8	0.0004369264761
C2	C8	0.0014565154185
C3	C8	4.8808795248e-05
O4	C8	7.8509261134e-05
C5	C8	0.0087366864324
C6	C8	0.041659535317
C7	C8	0.94741207789



N1	N9	0.00013580523135
C2	N9	0.00035614829319
C3	N9	1.1382137874e-05
O4	N9	4.1397553447e-05
C5	N9	0.0017355027298
C6	N9	0.011151089373
C7	N9	0.072493598139
C8	N9	0.95329946074
N1	N1	0.061218924428
C2	N1	0.90772319714
C3	N1	0.044510051835
O4	N1	0.0149769459
C5	N1	0.034062034281
C6	N1	0.010543176321
C7	N1	0.0011887904386
C8	N1	5.356754496e-05
N9	N1	2.8111618331e-05
N1	H11	0.0056605861989
C2	H11	0.041790865347
C3	H11	0.0058285411453
O4	H11	0.013587284914
C5	H11	0.94044643098
C6	H11	0.037641592303
C7	H11	0.0076737467919
C8	H11	0.00083644264591
N9	H11	7.5583906792e-05
N1	H11	0.0092264731788
N1	H12	0.022858478919
C2	H12	0.042392314074
C3	H12	0.0070177768263
O4	H12	0.0024433440622
C5	H12	0.94104281539
C6	H12	0.039587072073
C7	H12	0.008062323551
C8	H12	0.0008126703787
N9	H12	8.908045933e-05
N1	H12	0.0018824448021
H11	H12	0.041961829972
N1	H13	0.00072639655621
C2	H13	0.0071680956321
C3	H13	0.00043520115268
O4	H13	0.0012915311194
C5	H13	0.044152786176
C6	H13	0.94545436854
C7	H13	0.041755585526
C8	H13	0.0074168001837
N9	H13	0.0010625638801
N1	H13	0.008528901556

H11	H13	0.010746386732
H12	H13	0.0040735999793
N1	H14	0.00062102315339
C2	H14	0.0032364735199
C3	H14	0.0011735154454
O4	H14	0.033106371565
C5	H14	0.038501811471
C6	H14	0.93291488467
C7	H14	0.0373292348
C8	H14	0.0066907698917
N9	H14	0.0015515203083
N1	H14	0.00078437915353
H11	H14	0.0027154735061
H12	H14	0.010164414924
H13	H14	0.041026028939
N1	H15	9.8838948077e-05
C2	H15	0.00076216537325
C3	H15	4.1293152279e-05
O4	H15	0.0001961823261
C5	H15	0.0077109268065
C6	H15	0.0416450793
C7	H15	0.94389631243
C8	H15	0.041155427751
N9	H15	0.011561979599
N1	H15	0.0003905100889
H11	H15	0.0071547204918
H12	H15	0.00059094413271
H13	H15	0.011127121437
H14	H15	0.003392619009
N1	H16	6.9063581042e-05
C2	H16	0.00071740103545
C3	H16	0.00014904961997
O4	H16	0.00049507684453
C5	H16	0.0078242397423
C6	H16	0.040195974109
C7	H16	0.94292039162
C8	H16	0.039573069956
N9	H16	0.017077930847
N1	H16	6.8059802521e-05
H11	H16	0.00059715864082
H12	H16	0.007554205571
H13	H16	0.0035445120185
H14	H16	0.009890076662
H15	H16	0.04330678252
N1	H17	1.5998338055e-05
C2	H17	4.3259986938e-05
C3	H17	3.7340408817e-06
O4	H17	1.7084036482e-05

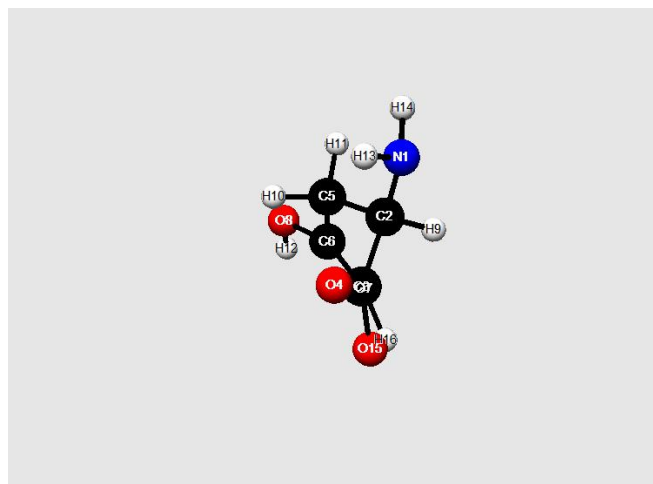
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C7	H17	0.040155297754
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N9	H17	0.064386325584
N1	H17	1.9249997751e-05
H11	H17	0.00036029971036
H12	H17	5.4401163767e-05
H13	H17	0.0070987741779
H14	H17	0.00053843164706
H15	H17	0.010869502602
H16	H17	0.0039545263348
N1	H18	2.9142424724e-05
C2	H18	4.2651083489e-05
C3	H18	5.5197362649e-06
O4	H18	5.6427284241e-05
C5	H18	0.00094806496713
C6	H18	0.0082068069837
C7	H18	0.041848621176
C8	H18	0.92713958755
N9	H18	0.076242767629
N1	H18	7.0931896371e-06
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H12	H18	0.00039968106325
H13	H18	0.00067468089961
H14	H18	0.0074686187169
H15	H18	0.0037323030914
H16	H18	0.010848440753
H17	H18	0.04260693808
N1	H19	3.1942394551e-05
C2	H19	9.3454192463e-05
C3	H19	2.9041873738e-06
O4	H19	5.9183388937e-06
C5	H19	0.00030795381737
C6	H19	0.0016394821388
C7	H19	0.0085287905004
C8	H19	0.021316578964
N9	H19	0.88826968632
N1	H19	4.8299669305e-06
H11	H19	1.0762594294e-05
H12	H19	1.1059495796e-05
H13	H19	3.8431392832e-05
H14	H19	5.1259508613e-05
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H16	H19	0.0005340078138
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H18	H19	0.001935142748
N1	C2	2.7078625818e-06

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O4	C2	2.4768222379e-06
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C6	C2	0.00047678312022
C7	C2	0.0041634762476
C8	C2	0.021591703725
N9	C2	0.88781021238
N1	C2	2.6335294377e-06
H11	C2	1.2637395105e-05
H12	C2	3.4509376499e-06
H13	C2	0.00025694737877
H14	C2	4.3027630605e-05
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H16	C2	0.00036484942417
H17	C2	0.0097614424887
H18	C2	0.0024314584736
H19	C2	0.018505320454
N1	H21	0.86729061735
C2	H21	0.020872608696
C3	H21	0.0014750490758
O4	H21	0.00062056740131
C5	H21	0.0060110470514
C6	H21	0.00068150454512
C7	H21	4.6510712552e-05
C8	H21	1.1903173575e-05
N9	H21	4.4409395082e-06
N1	H21	0.0086341308712
H11	H21	0.0024036598729
H12	H21	0.0015297341036
H13	H21	0.00020969873808
H14	H21	6.0019520017e-05
H15	H21	1.4980294714e-05
H16	H21	6.2451485081e-06
H17	H21	1.8574507703e-06
H18	H21	1.2953936394e-06
H19	H21	5.6080423614e-07
C2	H21	2.0981722826e-07
N1	H22	0.86344010435
C2	H22	0.020128727144
C3	H22	0.0066482315488
O4	H22	0.0021502055157
C5	H22	0.0022933497806
C6	H22	0.00023761968473
C7	H22	3.625664792e-05
C8	H22	8.7833674472e-06
N9	H22	3.5589778701e-06
N1	H22	0.0035931036255

H11	H22	0.00023177718316
H12	H22	0.0022691076329
H13	H22	4.013196155e-05
H14	H22	5.7644424262e-05
H15	H22	2.9293176286e-06
H16	H22	4.5409382848e-06
H17	H22	6.767426388e-07
H18	H22	1.0407481535e-06
H19	H22	6.2609096665e-07
C2	H22	1.0941844432e-07
H21	H22	0.01705315386
N1	O23	0.082479642601
C2	O23	0.083540233855
C3	O23	0.73623202479
O4	O23	0.27843222249
C5	O23	0.0084782952795
C6	O23	0.00054668210153
C7	O23	0.00016184935126
C8	O23	2.6911467963e-05
N9	O23	9.0627376276e-06
N1	O23	0.0091179004599
H11	O23	0.0008967743197
H12	O23	0.0021399878129
H13	O23	0.00012166532707
H14	O23	0.00073782464732
H15	O23	2.1464096366e-05
H16	O23	5.674118163e-05
H17	O23	4.6244938372e-06
H18	O23	1.1380034663e-05
H19	O23	3.3954142157e-06
C2	O23	1.8399936581e-06
H21	O23	0.0017566785574
H22	O23	0.0028572059257
N1	H24	0.04583531186
C2	H24	0.0022615023735
C3	H24	0.0062995772203
O4	H24	0.0077688312409
C5	H24	0.00064500294561
C6	H24	0.00010444340163
C7	H24	1.5215404005e-05
C8	H24	5.8461569329e-06
N9	H24	1.4801970156e-06
N1	H24	0.00012297368795
H11	H24	2.9204621191e-05
H12	H24	9.867171848e-05
H13	H24	5.8327518508e-06
H14	H24	4.2682495368e-05
H15	H24	1.2473369342e-06

H16	H24	2.6870576016e-06
H17	H24	1.7430957114e-07
H18	H24	6.8910724749e-07
H19	H24	3.6493510902e-07
C2	H24	6.5763853422e-08
H21	H24	0.00072273294595
H22	H24	0.00091811188137
O23	H24	0.48220786109

## ASPARTIC ACID



## HARTREE-FOCK

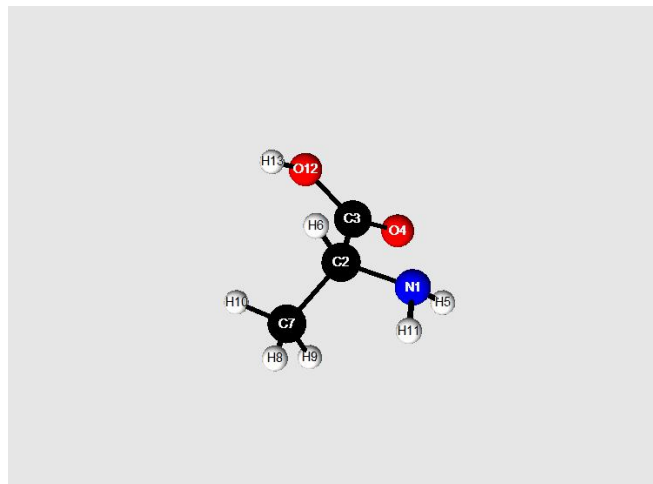
Atom A	Atom B	Delocalization index
N1	C2	0.98292963767
N1	C3	0.052143353227
C2	C3	0.85262038142
N1	O4	0.060741942429
C2	O4	0.097569045687
C3	O4	1.1082837467
N1	C5	0.080426424682
C2	C5	0.92871270224
C3	C5	0.044603923493
O4	C5	0.016300252307
N1	C6	0.010940112486
C2	C6	0.031016719604
C3	C6	0.0018437076093
O4	C6	0.00073525694603
C5	C6	0.90091734956
N1	O7	0.0028509212724
C2	O7	0.021476669983
C3	O7	0.0020731714134
O4	O7	0.0017841509715
C5	O7	0.096385345726
C6	O7	1.0775090647
N1	O8	0.0025723782036
C2	O8	0.008959146444
C3	O8	0.00061928022302
O4	O8	0.00036462991085
C5	O8	0.089926302432
C6	O8	0.72762484295
O7	O8	0.29092977749
N1	H9	0.059542820575
C2	H9	0.90741084172

C3	H9	0.034849271092
O4	H9	0.011343616162
C5	H9	0.038753664939
C6	H9	0.0039788249596
O7	H9	0.021355367587
O8	H9	0.00086281024169
N1	N1	0.0069647629018
C2	N1	0.032783398018
C3	N1	0.0060608508745
O4	N1	0.0067395404372
C5	N1	0.9346619008
C6	N1	0.04400214391
O7	N1	0.013308876771
O8	N1	0.01346581916
H9	N1	0.0088482809749
N1	H11	0.017414745296
C2	H11	0.032999342154
C3	H11	0.0075062374277
O4	H11	0.0026195902972
C5	H11	0.93176950214
C6	H11	0.045808689683
O7	H11	0.014142861555
O8	H11	0.015247916764
H9	H11	0.0019348018651
N1	H11	0.036324808345
N1	H12	0.00043443942421
C2	H12	0.0010371850798
C3	H12	4.0326138216e-05
O4	H12	2.8992723114e-05
C5	H12	0.006175160788
C6	H12	0.0081333482836
O7	H12	0.0097561275084
O8	H12	0.5332569459
H9	H12	2.0506105612e-05
N1	H12	0.00022742913766
H11	H12	0.00025960378087
N1	H13	0.81390695992
C2	H13	0.019773894188
C3	H13	0.0034239730651
O4	H13	0.028088849397
C5	H13	0.0019440514233
C6	H13	0.0002440541508
O7	H13	0.0003578270232
O8	H13	5.8248606922e-05
H9	H13	0.0074600578083
N1	H13	0.00055653127538
H11	H13	0.00031662509749
H12	H13	8.1756504739e-06



N1	H14	0.87430310926
C2	H14	0.021602960947
C3	H14	0.0068056468426
O4	H14	0.0031086080654
C5	H14	0.0074830728115
C6	H14	0.0004279878917
O7	H14	0.00023317773519
O8	H14	0.00011790509905
H9	H14	0.00098749810675
N1	H14	0.00031932479978
H11	H14	0.0061360008109
H12	H14	1.115400375e-05
H13	H14	0.015483184793
N1	O15	0.01123529423
C2	O15	0.089643366238
C3	O15	0.73651903925
O4	O15	0.27924018698
C5	O15	0.010526447914
C6	O15	0.0042778959789
O7	O15	0.058508739767
O8	O15	0.001458904362
H9	O15	0.015964436501
N1	O15	0.0011822127253
H11	O15	0.0014871152097
H12	O15	3.3329101127e-05
H13	O15	0.00095505316172
H14	O15	0.0018451639334
N1	H16	0.00028655521595
C2	H16	0.0022355599084
C3	H16	0.0059425959408
O4	H16	0.0077046337519
C5	H16	0.00040654117625
C6	H16	0.0012605908335
O7	H16	0.040915444448
O8	H16	0.0011395733997
H9	H16	0.001544314379
N1	H16	4.7751060598e-05
H11	H16	4.8078359877e-05
H12	H16	1.2784818831e-05
H13	H16	5.9123102564e-05
H14	H16	3.3569080482e-05
O15	H16	0.47005432164

## ALANINE



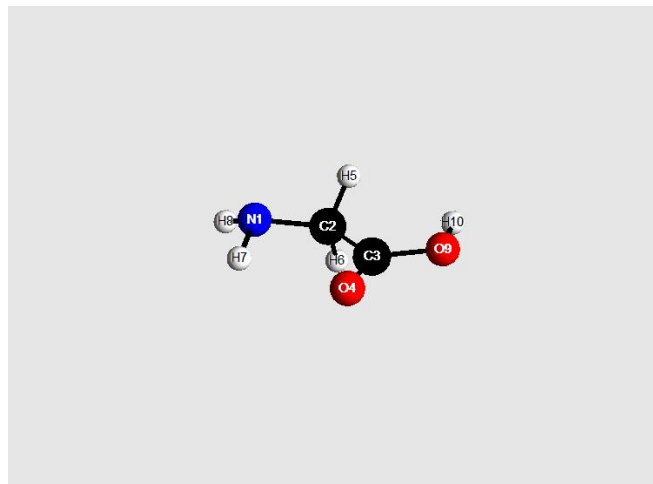
## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97797736052
N1	C3	0.05536889223
C2	C3	0.85741878104
N1	O4	0.053230315766
C2	O4	0.09401082454
C3	O4	1.1170636248
N1	H5	0.82414827032
C2	H5	0.019860448054
C3	H5	0.0033809144346
O4	H5	0.024993285198
N1	H6	0.063275458518
C2	H6	0.91323241675
C3	H6	0.037854912841
O4	H6	0.011860291091
H5	H6	0.0081938791569
N1	C7	0.076561683506
C2	C7	0.94097533784
C3	C7	0.046763770293
O4	C7	0.018726092172
H5	C7	0.0021408871867
H6	C7	0.041129684315
N1	H8	0.010684450183
C2	H8	0.040781604595
C3	H8	0.0093560204679
O4	H8	0.0037622650937
H5	H8	0.00025755131021
H6	H8	0.0040272860678
C7	H8	0.96111222142
N1	H9	0.011907871162
C2	H9	0.039081743532

C3	H9	0.0047235193386
O4	H9	0.0075939315219
H5	H9	0.0011004693795
H6	H9	0.010632459141
C7	H9	0.95718268491
H8	H9	0.040928365481
N1	N1	0.01565229887
C2	N1	0.039392937855
C3	N1	0.0037699296182
O4	N1	0.0010754512168
H5	N1	0.00033631096258
H6	N1	0.003362518659
C7	N1	0.96288277448
H8	N1	0.041920082871
H9	N1	0.040698497978
N1	H11	0.87555779167
C2	H11	0.021469654384
C3	H11	0.0070573468357
O4	H11	0.0027691066585
H5	H11	0.015745907508
H6	H11	0.0010509756212
C7	H11	0.0072509181177
H8	H11	0.0044045432168
H9	H11	0.00053134827981
N1	H11	0.00063845053593
N1	O12	0.011185051197
C2	O12	0.08894423271
C3	O12	0.71570281842
O4	O12	0.27534887
H5	O12	0.00093373083521
H6	O12	0.02111844599
C7	O12	0.015071322826
H8	O12	0.0021090876834
H9	O12	0.0010222624167
N1	O12	0.011319248569
H11	O12	0.0018105722716
N1	H13	0.0007973904162
C2	H13	0.004748560406
C3	H13	0.0072283599749
O4	H13	0.010327642493
H5	H13	0.00016274347868
H6	H13	0.0051477512421
C7	H13	0.00077783313094
H8	H13	9.6451194585e-05
H9	H13	0.00010265843637
N1	H13	0.00082183909885
H11	H13	3.853160498e-05
O12	H13	0.56401494799



## GLYCINE

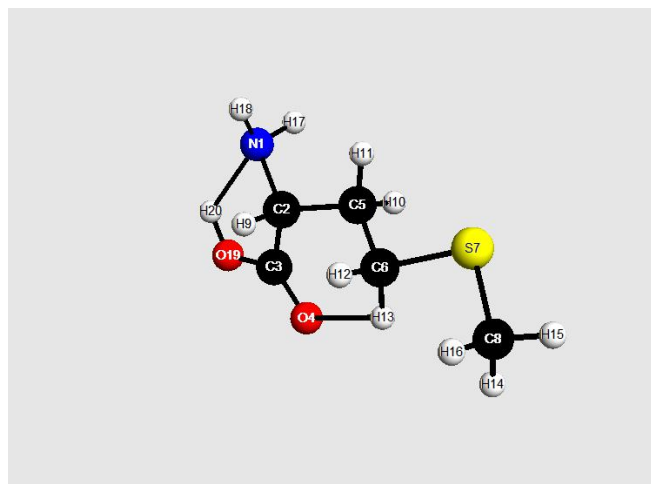


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	1.0022004108
N1	C3	0.05203165541
C2	C3	0.87273127585
N1	O4	0.052786198157
C2	O4	0.098445099765
C3	O4	1.1219839913
N1	H5	0.06189290575
C2	H5	0.92391599792
C3	H5	0.040781258517
O4	H5	0.013920928318
N1	H6	0.069243934596
C2	H6	0.92222411725
C3	H6	0.047896371899
O4	H6	0.015866459072
H5	H6	0.04038039221
N1	H7	0.81944355419
C2	H7	0.020066304876
C3	H7	0.0038027424998
O4	H7	0.026489656201
H5	H7	0.0075690808748
H6	H7	0.0013349077453
N1	H8	0.87645488115
C2	H8	0.022230095164
C3	H8	0.0063338478549
O4	H8	0.0026582895203
H5	H8	0.0010254818381
H6	H8	0.0039149087808
H7	H8	0.015561258681
N1	O9	0.013772478187
C2	O9	0.095772016427

C3	O9	0.71538037115
O4	O9	0.2738680849
H5	O9	0.01864471972
H6	O9	0.01289471595
H7	O9	0.0010036904476
H8	O9	0.001674462798
N1	N1	0.00082065800359
C2	N1	0.0048555999978
C3	N1	0.0072995496999
O4	N1	0.010425486728
H5	N1	0.0037596791227
H6	N1	0.00063248695941
H7	N1	0.0001491947813
H8	N1	3.8257525476e-05
O9	N1	0.56694999155

# METHIONINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.94354774605
N1	C3	0.055737288525
C2	C3	0.85473739176
N1	O4	0.014160414798
C2	O4	0.10176209969
C3	O4	1.106194472
N1	C5	0.073064211622
C2	C5	0.93639277749
C3	C5	0.03342790362
O4	C5	0.022920428634
N1	C6	0.012093872149
C2	C6	0.038789732942
C3	C6	0.0018910910359
O4	C6	0.022514267403
C5	C6	0.97442912658
N1	S7	0.0024490461555
C2	S7	0.011888819413
C3	S7	0.00063424854896
O4	S7	0.0037793402802
C5	S7	0.062913451746
C6	S7	1.0697151025
N1	C8	0.00051141824582
C2	C8	0.0019267789541
C3	C8	8.448753361e-05
O4	C8	0.00011848861783
C5	C8	0.0093449295271
C6	C8	0.042482105223
S7	C8	1.0957756795
N1	H9	0.060531055411
C2	H9	0.90847188213

C3	H9	0.044033310915
O4	H9	0.015428764293
C5	H9	0.034535025292
C6	H9	0.0093365781686
S7	H9	0.0018894636659
C8	H9	6.7713332313e-05
N1	N1	0.0064981221079
C2	N1	0.04030967943
C3	N1	0.0052364323964
O4	N1	0.0093248340185
C5	N1	0.94029133401
C6	N1	0.039784893759
S7	N1	0.015364700527
C8	N1	0.00082263150591
H9	N1	0.0092596015264
N1	H11	0.021420571583
C2	H11	0.041010787723
C3	H11	0.0071444895873
O4	H11	0.0022154946934
C5	H11	0.93795377027
C6	H11	0.041342430728
S7	H11	0.021157410411
C8	H11	0.0014962166077
H9	H11	0.002227079057
N1	H11	0.040052755151
N1	H12	0.00080365465414
C2	H12	0.0076703388989
C3	H12	0.00044277553919
O4	H12	0.0014675478004
C5	H12	0.038979850739
C6	H12	0.94876609448
S7	H12	0.063456256976
C8	H12	0.005125084939
H9	H12	0.0083996356323
N1	H12	0.010221501189
H11	H12	0.0028603847825
N1	H13	0.00054557676703
C2	H13	0.0020115785168
C3	H13	0.00087128601551
O4	H13	0.034779970875
C5	H13	0.033774698863
C6	H13	0.92998852936
S7	H13	0.053512061291
C8	H13	0.0068717888427
H9	H13	0.00039220679985
N1	H13	0.0033290024748
H11	H13	0.0095546974145
H12	H13	0.035470865721

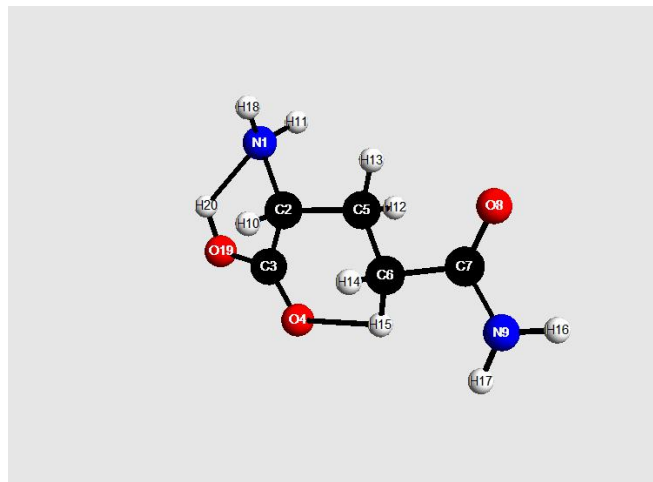


N1	H14	2.758198076e-05
C2	H14	5.721370135e-05
C3	H14	8.8183324549e-06
O4	H14	6.4417764775e-05
C5	H14	0.00063199797534
C6	H14	0.0056336669973
S7	H14	0.062937764346
C8	H14	0.96222919907
H9	H14	5.0675556543e-06
N1	H14	5.5854569744e-05
H11	H14	0.00040339091968
H12	H14	0.00036416685324
H13	H14	0.0048008649227
N1	H15	0.00016830886623
C2	H15	0.00045507539783
C3	H15	1.4012353192e-05
O4	H15	3.0606875154e-05
C5	H15	0.001809295183
C6	H15	0.0099989716824
S7	H15	0.052477331457
C8	H15	0.96655895521
H9	H15	2.2413129563e-05
N1	H15	4.5923844663e-05
H11	H15	6.8636726862e-05
H12	H15	0.00058254856378
H13	H15	0.00074383440376
H14	H15	0.037558235481
N1	H16	1.9759589741e-05
C2	H16	6.9791098975e-05
C3	H16	4.6686377932e-06
O4	H16	1.3377271279e-05
C5	H16	0.00073391025618
C6	H16	0.0054367212683
S7	H16	0.063612818931
C8	H16	0.96419490303
H9	H16	2.6758685972e-05
N1	H16	0.00034074069395
H11	H16	7.2837401309e-05
H12	H16	0.0040083931461
H13	H16	0.00042162058563
H14	H16	0.038422127797
H15	H16	0.038114461286
N1	H17	0.86420080951
C2	H17	0.020798885757
C3	H17	0.0013781955555
O4	H17	0.00060761746448
C5	H17	0.0064635498896
C6	H17	0.00068534955568

S7	H17	8.9777324408e-05
C8	H17	1.522347629e-05
H9	H17	0.0084325930761
N1	H17	0.0029230978311
H11	H17	0.0012973846384
H12	H17	0.00023046291104
H13	H17	3.5918064361e-05
H14	H17	9.700143783e-07
H15	H17	3.446525427e-06
H16	H17	2.3017739467e-06
N1	H18	0.86050340898
C2	H18	0.020094309783
C3	H18	0.0064259030423
O4	H18	0.0021115466836
C5	H18	0.0022296691856
C6	H18	0.00025269050453
S7	H18	6.5874744197e-05
C8	H18	1.2197941519e-05
H9	H18	0.0036916893793
N1	H18	0.00024169259379
H11	H18	0.0020572864133
H12	H18	3.6994217929e-05
H13	H18	5.633128677e-05
H14	H18	1.1930959769e-06
H15	H18	3.3618280025e-06
H16	H18	9.3046241964e-07
H17	H18	0.016838402831
N1	O19	0.083769761039
C2	O19	0.083461831133
C3	O19	0.73820490481
O4	O19	0.27853343906
C5	O19	0.0083637330287
C6	O19	0.00062362579317
S7	O19	0.0003262695552
C8	O19	4.7647566024e-05
H9	O19	0.008535975951
N1	O19	0.00079096618426
H11	O19	0.0021069307358
H12	O19	0.00013990052443
H13	O19	0.00074053228116
H14	O19	1.3696973887e-05
H15	O19	1.0637259304e-05
H16	O19	6.6235426991e-06
H17	O19	0.0017775332874
H18	O19	0.0028516081877
N1	C2	0.047028974688
C2	C2	0.0022581583664
C3	C2	0.006252547256

O4	C2	0.0076622535193
C5	C2	0.00065555972878
C6	C2	0.00011550296108
S7	C2	2.2825563026e-05
C8	C2	7.8466193117e-06
H9	C2	0.00010879279216
N1	C2	2.4428898665e-05
H11	C2	9.5509354083e-05
H12	C2	5.7306726609e-06
H13	C2	4.85399558e-05
H14	C2	7.3840121081e-07
H15	C2	1.786405841e-06
H16	C2	2.6138441523e-07
H17	C2	0.0007237099374
H18	C2	0.0009429529004
O19	C2	0.47871568874

## GLUTAMINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.94331930981
N1	C3	0.055947545543
C2	C3	0.85508395419
N1	O4	0.014069613277
C2	O4	0.10105138392
C3	O4	1.1013613743
N1	C5	0.073228113027
C2	C5	0.93965596143
C3	C5	0.033884133001
O4	C5	0.022469783632
N1	C6	0.012141945346
C2	C6	0.039288146257
C3	C6	0.001916558833
O4	C6	0.023438529239
C5	C6	0.96686155927
N1	C7	0.0016163154885
C2	C7	0.0071502991074
C3	C7	0.00019894967189
O4	C7	0.0019325210994
C5	C7	0.034326273224
C6	C7	0.89602874624
N1	O8	0.00034767507464
C2	O8	0.0033393863123
C3	O8	0.00043484474813
O4	O8	0.0010138102893
C5	O8	0.032943780203
C6	O8	0.10387249843
C7	O8	1.1039329888
N1	N9	0.00054014773582
C2	N9	0.0013588706071

C3	N9	3.6196725203e-05
O4	N9	0.00027198322533
C5	N9	0.0088286321637
C6	N9	0.087069986356
C7	N9	0.88631216642
O8	N9	0.26901637404
N1	N1	0.060617314183
C2	N1	0.9087154987
C3	N1	0.044732721962
O4	N1	0.015550373898
C5	N1	0.034460458503
C6	N1	0.0092255364519
C7	N1	0.0007538125457
O8	N1	0.00046602623658
N9	N1	0.00019855785143
N1	H11	0.86346825638
C2	H11	0.020741751063
C3	H11	0.0013658112956
O4	H11	0.00060674692499
C5	H11	0.0067479165433
C6	H11	0.00070426854217
C7	H11	4.2164582516e-05
O8	H11	4.0523547388e-05
N9	H11	1.6441055725e-05
N1	H11	0.008359362508
N1	H12	0.0068320454925
C2	H12	0.041579621346
C3	H12	0.0053169098886
O4	H12	0.0088649202604
C5	H12	0.94255213825
C6	H12	0.040616046387
C7	H12	0.0035226251442
O8	H12	0.0070767197693
N9	H12	0.00069717885082
N1	H12	0.0095736464527
H11	H12	0.0031724262266
N1	H13	0.019947130482
C2	H13	0.03900406301
C3	H13	0.0070129339998
O4	H13	0.0021603112059
C5	H13	0.93072321034
C6	H13	0.037878011823
C7	H13	0.0035650246141
O8	H13	0.028215351058
N9	H13	0.00098604724583
N1	H13	0.0021970719065
H11	H13	0.0012497895592
H12	H13	0.038601400818

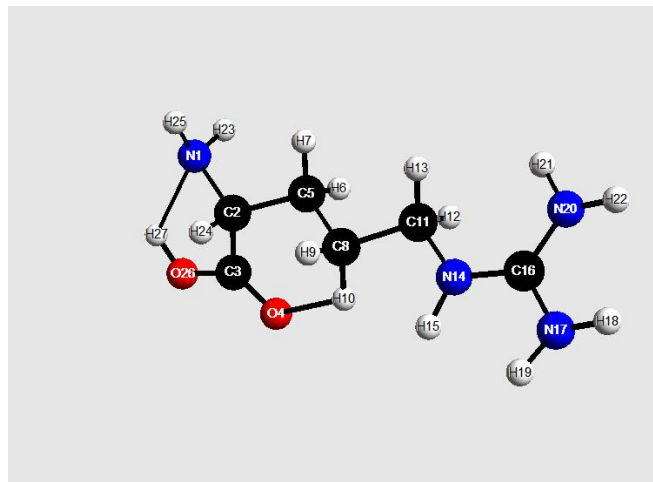
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C2	H14	0.007512287044
C3	H14	0.0004378469079
O4	H14	0.0014557172502
C5	H14	0.038492369162
C6	H14	0.94162496151
C7	H14	0.046805763453
O8	H14	0.015132701996
N9	H14	0.012441809903
N1	H14	0.0078228296114
H11	H14	0.000226519697
H12	H14	0.010363779734
H13	H14	0.0028833050672
N1	H15	0.00054578186393
C2	H15	0.0021157330549
C3	H15	0.00093290681
O4	H15	0.037784922832
C5	H15	0.034594331258
C6	H15	0.92969766157
C7	H15	0.034742499179
O8	H15	0.011626751079
N9	H15	0.017511612449
N1	H15	0.00037520948218
H11	H15	3.749116073e-05
H12	H15	0.0032373614676
H13	H15	0.00921017372
H14	H15	0.037782010117
N1	H16	0.00012548158965
C2	H16	0.00027511229836
C3	H16	5.7383474461e-06
O4	H16	1.3146574238e-05
C5	H16	0.0013209365279
C6	H16	0.0077078369733
C7	H16	0.014933930872
O8	H16	0.011793884296
N9	H16	0.80148277881
N1	H16	1.9610695418e-05
H11	H16	2.1839936687e-06
H12	H16	3.2739645198e-05
H13	H16	3.8775576845e-05
H14	H16	0.00036527612211
H15	H16	0.00064003988516
N1	H17	1.8422066646e-05
C2	H17	4.2548516976e-05
C3	H17	5.0085256074e-06
O4	H17	5.5740533544e-05
C5	H17	0.00059425593372
C6	H17	0.0055541392913

C7	H17	0.013991607124
O8	H17	0.014542028893
N9	H17	0.81377066532
N1	H17	3.6676632901e-06
H11	H17	8.7976980495e-07
H12	H17	2.978900247e-05
H13	H17	0.00021706860514
H14	H17	0.00029022784651
H15	H17	0.0051705908251
H16	H17	0.014709230105
N1	H18	0.85973980098
C2	H18	0.020040366087
C3	H18	0.0063554640111
O4	H18	0.0020734743166
C5	H18	0.0022233377081
C6	H18	0.00025287344591
C7	H18	3.2329007427e-05
O8	H18	1.9853542161e-05
N9	H18	1.0990179272e-05
N1	H18	0.0037857423067
H11	H18	0.016747268558
H12	H18	0.00025132797664
H13	H18	0.0018655386832
H14	H18	3.7678646519e-05
H15	H18	5.16955106e-05
H16	H18	2.1558658062e-06
H17	H18	6.2310425559e-07
N1	O19	0.084855540315
C2	O19	0.082885167828
C3	O19	0.74057500587
O4	O19	0.2787964336
C5	O19	0.008329637581
C6	O19	0.00063078915862
C7	O19	0.00012971095608
O8	O19	0.00017125008971
N9	O19	2.832660154e-05
N1	O19	0.0084609160349
H11	O19	0.0017855343776
H12	O19	0.00079491556916
H13	O19	0.002012267716
H14	O19	0.00013623826724
H15	O19	0.00079598297444
H16	O19	4.4611406961e-06
H17	O19	1.1097587045e-05
H18	O19	0.0028804856026
N1	C2	0.048248819889
C2	C2	0.002274845311
C3	C2	0.0062624177382

O4	C2	0.0075748352424
C5	C2	0.00066072727727
C6	C2	0.00011819814451
C7	C2	1.1878790765e-05
O8	C2	6.6298925729e-06
N9	C2	5.8686225464e-06
N1	C2	0.00010759373047
H11	C2	0.00073994120846
H12	C2	2.4102394241e-05
H13	C2	8.9675673701e-05
H14	C2	6.2980974129e-06
H15	C2	5.179369753e-05
H16	C2	1.3138889049e-06
H17	C2	5.2098420784e-07
H18	C2	0.00097276302464
O19	C2	0.47585649525



## ARGININE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.94840031684
N1	C3	0.056145534449
C2	C3	0.85337882142
N1	O4	0.014218482464
C2	O4	0.10192358521
C3	O4	1.1044378052
N1	C5	0.073313498372
C2	C5	0.93781841878
C3	C5	0.033356725409
O4	C5	0.024783675995
N1	H6	0.0061177189841
C2	H6	0.040232597827
C3	H6	0.0055030174948
O4	H6	0.01228015149
C5	H6	0.94090553033
N1	H7	0.021480378392
C2	H7	0.040734470424
C3	H7	0.0070430797672
O4	H7	0.0024158689779
C5	H7	0.94171463585
H6	H7	0.040999771599
N1	C8	0.011718661028
C2	C8	0.037926457576
C3	C8	0.0018746505377
O4	C8	0.021771861021
C5	C8	0.96526306856
H6	C8	0.038738275179
H7	C8	0.040478658336
N1	H9	0.00073093371354
C2	H9	0.0068199611525

C3	H9	0.00040201471651
O4	H9	0.0013696753547
C5	H9	0.040083391785
H6	H9	0.010274899685
H7	H9	0.0036728770713
C8	H9	0.94415551428
N1	N1	0.00055811527321
C2	N1	0.0028214044836
C3	N1	0.0011626190968
O4	N1	0.037916755912
C5	N1	0.035119376943
H6	N1	0.0026960506352
H7	N1	0.0097261118389
C8	N1	0.92751260799
H9	N1	0.037969805007
N1	C11	0.0018084136773
C2	C11	0.008372834784
C3	C11	0.00030709330835
O4	C11	0.0017961334994
C5	C11	0.045449802697
H6	C11	0.0072019529923
H7	C11	0.007745931354
C8	C11	0.94593352156
H9	C11	0.042504707494
N1	C11	0.038347274459
N1	H12	9.7663598594e-05
C2	H12	0.0007806763083
C3	H12	3.8034915379e-05
O4	H12	0.00020044444264
C5	H12	0.0072345705259
H6	H12	0.0066454218277
H7	H12	0.00058200589909
C8	H12	0.034560129183
H9	H12	0.010017436751
N1	H12	0.0032049518186
C11	H12	0.91836640074
N1	H13	6.4032149127e-05
C2	H13	0.00071247716352
C3	H13	0.00015108513146
O4	H13	0.00051287531249
C5	H13	0.0072566911106
H6	H13	0.00054984610131
H7	H13	0.0071466457575
C8	H13	0.034640202259
H9	H13	0.0039598567953
N1	H13	0.0089486884181
C11	H13	0.9153372829
H12	H13	0.037568589287

N1	N14	0.00056202477406
C2	N14	0.0016562153988
C3	N14	5.6439238934e-05
O4	N14	0.00019025045933
C5	N14	0.010803709418
H6	N14	0.001155463369
H7	N14	0.0011556107243
C8	N14	0.074071571023
H9	N14	0.013245388742
N1	N14	0.010822086002
C11	N14	0.83704930237
H12	N14	0.068964873196
H13	N14	0.068064376851
N1	H15	2.3476183603e-05
C2	H15	2.9576002453e-05
C3	H15	5.4498227354e-06
O4	H15	8.3818566623e-05
C5	H15	0.00084959117077
H6	H15	0.00011304951038
H7	H15	0.00024636019442
C8	H15	0.0077918062757
H9	H15	0.0021588360215
N1	H15	0.003566079524
C11	H15	0.014505749354
H12	H15	0.0023658598947
H13	H15	0.004658067287
N14	H15	0.77295835391
N1	C16	7.750666466e-05
C2	C16	0.00018351505691
C3	C16	6.0686746151e-06
O4	C16	1.6119183727e-05
C5	C16	0.0010435885011
H6	C16	7.6189598061e-05
H7	C16	0.00010186590173
C8	C16	0.0048618200154
H9	C16	0.00048271515282
N1	C16	0.00034629040359
C11	C16	0.017027993903
H12	C16	0.0046055662362
H13	C16	0.0040419248916
N14	C16	0.98384428232
H15	C16	0.015037906757
N1	N17	3.4516927451e-05
C2	N17	7.682294278e-05
C3	N17	4.4706690129e-06
O4	N17	9.212963141e-05
C5	N17	0.00039387839626
H6	N17	0.00016067734641

H7	N17	0.00046437344529
C8	N17	0.0014526601632
H9	N17	0.0020763362106
N1	N17	0.00050667526018
C11	N17	0.0097896585357
H12	N17	0.0043764396356
H13	N17	0.0069648960079
N14	N17	0.18362113023
H15	N17	0.014592071175
C16	N17	1.0187466764
N1	H18	2.1015013646e-05
C2	H18	2.9278565963e-05
C3	H18	2.4959297683e-06
O4	H18	0.00013606653982
C5	H18	0.00015564634436
H6	H18	0.00015115608699
H7	H18	0.0006597508112
C8	H18	0.00072687837209
H9	H18	0.0029205535351
N1	H18	0.00061633122668
C11	H18	0.002310786288
H12	H18	0.002937153105
H13	H18	0.0079572924151
N14	H18	0.020528099433
H15	H18	0.0080934913525
C16	H18	0.019435444458
N17	H18	0.78373324521
N1	H19	7.9139084265e-06
C2	H19	6.099156199e-06
C3	H19	1.033034289e-06
O4	H19	5.7854073921e-05
C5	H19	6.3593022029e-05
H6	H19	6.3658755765e-05
H7	H19	0.00027041822884
C8	H19	0.00024257071348
H9	H19	0.0012296064613
N1	H19	0.00026530822903
C11	H19	0.0008317353581
H12	H19	0.0013216979969
H13	H19	0.0032624172652
N14	H19	0.013874424218
H15	H19	0.0062608067654
C16	H19	0.01759789841
N17	H19	0.79656531929
H18	H19	0.050151101639
N1	C2	2.228397322e-05
C2	C2	4.1058161508e-05
C3	C2	3.6816984632e-06

O4	C2	0.00011737779175
C5	C2	0.00020854943468
H6	C2	0.00014190170473
H7	C2	0.00048895375329
C8	C2	0.0030195773959
H9	C2	0.0024291926803
N1	C2	0.00089375756947
C11	C2	0.021325785028
H12	C2	0.011437603996
H13	C2	0.018510482802
N14	C2	0.17807131306
H15	C2	0.013962722388
C16	C2	1.0065415546
N17	C2	0.21743527529
H18	C2	0.075681128438
H19	C2	0.036136645656
N1	H21	8.3405803221e-06
C2	H21	1.5497647715e-05
C3	H21	2.1824254327e-06
O4	H21	4.3681011875e-05
C5	H21	6.5263242292e-05
H6	H21	3.8900986568e-05
H7	H21	0.00015448657297
C8	H21	0.0013932871103
H9	H21	0.00064653062744
N1	H21	0.00032245509384
C11	H21	0.0099910319507
H12	H21	0.0036131366141
H13	H21	0.009762415983
N14	H21	0.0076309208584
H15	H21	0.0017735749058
C16	H21	0.015177225346
N17	H21	0.020208767695
H18	H21	0.018876269925
H19	H21	0.0082308800845
C2	H21	0.77457336688
N1	H22	1.777812238e-05
C2	H22	1.1693201883e-05
C3	H22	1.9576243374e-06
O4	H22	0.00014998270774
C5	H22	0.00013174087595
H6	H22	0.00016255619655
H7	H22	0.00071849181843
C8	H22	0.00061018306907
H9	H22	0.0031841471719
N1	H22	0.0006677596423
C11	H22	0.0020603458618
H12	H22	0.0032245698778

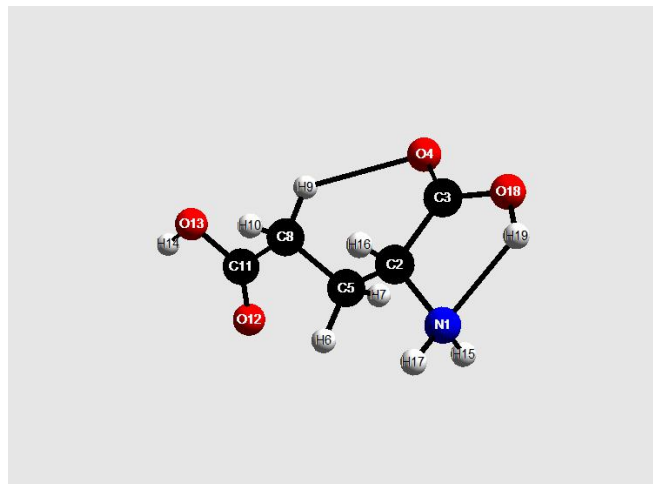
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N14	H22	0.021647583053
H15	H22	0.009108305554
C16	H22	0.019033340878
N17	H22	0.078730169121
H18	H22	0.11653114227
H19	H22	0.04509063623
C2	H22	0.78184164915
H21	H22	0.029706205835
N1	H23	0.8634305008
C2	H23	0.020894716743
C3	H23	0.0014305693965
O4	H23	0.00060837471728
C5	H23	0.0058632185485
H6	H23	0.0025088736025
H7	H23	0.0012228064374
C8	H23	0.00062878388605
H9	H23	0.00020127025532
N1	H23	4.1589563303e-05
C11	H23	4.70887438e-05
H12	H23	1.4919563673e-05
H13	H23	6.0484609742e-06
N14	H23	1.6983923705e-05
H15	H23	2.3854103768e-06
C16	H23	2.3592800847e-06
N17	H23	6.8454592498e-06
H18	H23	9.2786533254e-06
H19	H23	3.8965677249e-06
C2	H23	7.1808956068e-06
H21	H23	2.0552195881e-06
H22	H23	1.0179866152e-05
N1	H24	0.060486535554
C2	H24	0.90804612199
C3	H24	0.043424841042
O4	H24	0.01497579108
C5	H24	0.034852926514
H6	H24	0.0091955349215
H7	H24	0.0020205043111
C8	H24	0.0096854186095
H9	H24	0.0076734547874
N1	H24	0.00054920665464
C11	H24	0.0010452163473
H12	H24	0.00034544539654
H13	H24	6.1927265497e-05
N14	H24	0.00010192675192
H15	H24	2.0281153806e-05
C16	H24	1.4415358606e-05
N17	H24	6.5447138357e-05

H18	H24	9.6956659065e-05
H19	H24	4.0120603231e-05
C2	H24	7.3932792349e-05
H21	H24	2.1525932541e-05
H22	H24	0.0001062433975
H23	H24	0.0085530867927
N1	H25	0.85799912285
C2	H25	0.020116130194
C3	H25	0.0065324182825
O4	H25	0.0021401345353
C5	H25	0.0021887469343
H6	H25	0.00022389119994
H7	H25	0.0020070819497
C8	H25	0.0002309903444
H9	H25	3.7672932584e-05
N1	H25	5.185984786e-05
C11	H25	3.5563273285e-05
H12	H25	3.9063453692e-06
H13	H25	8.4541397553e-06
N14	H25	1.7936156632e-05
H15	H25	4.6649130936e-06
C16	H25	4.1148632251e-06
N17	H25	3.0667816576e-05
H18	H25	4.6667496729e-05
H19	H25	1.915226752e-05
C2	H25	3.2075436581e-05
H21	H25	9.0991710971e-06
H22	H25	5.1070374323e-05
H23	H25	0.016750957801
H24	H25	0.0035584998183
N1	O26	0.081264792353
C2	O26	0.083842259902
C3	O26	0.74060075731
O4	O26	0.2779012952
C5	O26	0.0085498617534
H6	O26	0.00086376470006
H7	O26	0.0021237550548
C8	O26	0.00060620227624
H9	O26	0.00012894114501
N1	O26	0.00082327797952
C11	O26	0.00016514023387
H12	O26	2.158172725e-05
H13	O26	6.1390254548e-05
N14	O26	3.6684341407e-05
H15	O26	9.8835842174e-06
C16	O26	3.6157304304e-06
N17	O26	6.1092443257e-06
H18	O26	4.3915694165e-06

H19	O26	5.5372423826e-06
C2	O26	6.459676045e-06
H21	O26	3.426313057e-06
H22	O26	4.4812932757e-06
H23	O26	0.0017281804087
H24	O26	0.0088575753186
H25	O26	0.0027312870883
N1	H27	0.044007083574
C2	H27	0.0022259547939
C3	H27	0.0063021275641
O4	H27	0.0077507546918
C5	H27	0.00064483051168
H6	H27	2.8221199117e-05
H7	H27	9.386464043e-05
C8	H27	0.00010659721943
H9	H27	6.3606834217e-06
N1	H27	4.8773950285e-05
C11	H27	1.4784241058e-05
H12	H27	1.2813849412e-06
H13	H27	2.9174180833e-06
N14	H27	6.7755413983e-06
H15	H27	4.5464919073e-07
C16	H27	7.7614930114e-07
N17	H27	5.968348857e-07
H18	H27	5.0912166922e-07
H19	H27	2.1028451876e-07
C2	H27	4.2595361644e-07
H21	H27	1.5009387091e-07
H22	H27	4.6451917456e-07
H23	H27	0.00068053506868
H24	H27	0.00011538750143
H25	H27	0.00086070410519
O26	H27	0.48072340197



## GLUTAMIC ACID



## HARTREE-FOCK

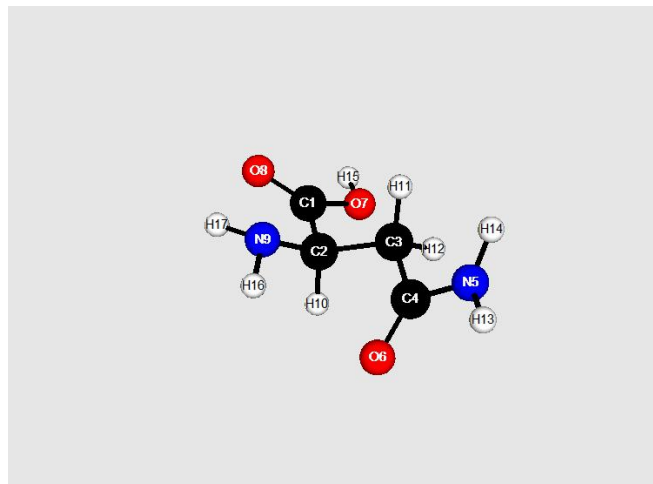
Atom A	Atom B	Delocalization index
N1	C2	0.94398859068
N1	C3	0.055751962495
C2	C3	0.85452500592
N1	O4	0.01412773254
C2	O4	0.10149385879
C3	O4	1.1051409564
N1	C5	0.073297643336
C2	C5	0.93939003382
C3	C5	0.03364747075
O4	C5	0.02294887996
N1	H6	0.020674568291
C2	H6	0.040033467732
C3	H6	0.0071632316695
O4	H6	0.0022370175016
C5	H6	0.9363919723
N1	H7	0.0066146526542
C2	H7	0.040050514153
C3	H7	0.005216286739
O4	H7	0.0092514311823
C5	H7	0.93906648305
H6	H7	0.038996890091
N1	C8	0.012038233657
C2	C8	0.039114393495
C3	C8	0.001947819618
O4	C8	0.023774146785
C5	C8	0.96842020625
H6	C8	0.040022078519
H7	C8	0.039266791767
N1	H9	0.00051673856001
C2	H9	0.0021185808816

C3	H9	0.00092234117029
O4	H9	0.03608800699
C5	H9	0.032221039366
H6	H9	0.0092928545925
H7	H9	0.0029827065185
C8	H9	0.9175089599
N1	N1	0.00075980636892
C2	N1	0.0069719060151
C3	N1	0.00040774888212
O4	N1	0.001355468104
C5	N1	0.037308780215
H6	N1	0.0029006455481
H7	N1	0.010001367638
C8	N1	0.93928433632
H9	N1	0.035700652022
N1	C11	0.0016353718806
C2	C11	0.0071342239328
C3	C11	0.00021177813884
O4	C11	0.0019783838725
C5	C11	0.034921036682
H6	C11	0.0040710351903
H7	C11	0.0029527559198
C8	C11	0.90010335503
H9	C11	0.041534316613
N1	C11	0.046811684268
N1	O12	0.00026155134953
C2	O12	0.0032788192142
C3	O12	0.00033446692731
O4	O12	0.00085998061698
C5	O12	0.031646417125
H6	O12	0.018139181788
H7	O12	0.012135741451
C8	O12	0.096930175703
H9	O12	0.012805039356
N1	O12	0.014474492065
C11	O12	1.1015204239
N1	O13	0.00056186030992
C2	O13	0.001385857583
C3	O13	3.8230958466e-05
O4	O13	0.00033448339329
C5	O13	0.0095078089462
H6	O13	0.00091323190516
H7	O13	0.00079398326927
C8	O13	0.090241794624
H9	O13	0.013558953477
N1	O13	0.014939478904
C11	O13	0.71646819122
O12	O13	0.29380442288

N1	H14	9.6488721671e-05
C2	H14	0.00020984162926
C3	H14	4.7394127518e-06
O4	H14	1.528072934e-05
C5	H14	0.0010894114008
H6	H14	2.5232833723e-05
H7	H14	2.4662053552e-05
C8	H14	0.0062994861246
H9	H14	0.00024171481067
N1	H14	0.00027365814403
C11	H14	0.0082539120029
O12	H14	0.010636202223
O13	H14	0.54519276117
N1	H15	0.86305093866
C2	H15	0.02071735605
C3	H15	0.0013705616993
O4	H15	0.00060284580897
C5	H15	0.0065494742982
H6	H15	0.0012407159031
H7	H15	0.0029837956953
C8	H15	0.00067822814955
H9	H15	3.3792177988e-05
N1	H15	0.00021298382767
C11	H15	3.8471279215e-05
O12	H15	4.4775740684e-05
O13	H15	1.7088136069e-05
H14	H15	1.9660060853e-06
N1	H16	0.060773135548
C2	H16	0.90919433353
C3	H16	0.044303636543
O4	H16	0.015467362092
C5	H16	0.034662938814
H6	H16	0.0022096671311
H7	H16	0.0093512680973
C8	H16	0.0091505005041
H9	H16	0.00035754020077
N1	H16	0.0073946704826
C11	H16	0.00073999810654
O12	H16	0.00058191836748
O13	H16	0.00013841131105
H14	H16	1.1121933581e-05
H15	H16	0.0084287462747
N1	H17	0.86049974926
C2	H17	0.02009710129
C3	H17	0.0064124144824
O4	H17	0.0021041775875
C5	H17	0.0022285810391
H6	H17	0.0019679579728

H7	H17	0.00024331861451
C8	H17	0.00024957664785
H9	H17	5.1169868304e-05
N1	H17	3.5416750115e-05
C11	H17	3.2905403182e-05
O12	H17	1.7092405417e-05
O13	H17	1.3786742578e-05
H14	H17	1.7431887135e-06
H15	H17	0.016781723741
H16	H17	0.0037283858245
N1	O18	0.083727200306
C2	O18	0.083181006732
C3	O18	0.73963370517
O4	O18	0.27839152122
C5	O18	0.0083656396354
H6	O18	0.002085839447
H7	O18	0.0007822250715
C8	O18	0.00063750517486
H9	O18	0.00077088553421
N1	O18	0.0001271441208
C11	O18	0.00013283771581
O12	O18	0.00014235988192
O13	O18	3.7174830791e-05
H14	O18	3.3619506394e-06
H15	O18	0.0017679692191
H16	O18	0.0085580153967
H17	O18	0.0028440518721
N1	H19	0.047026985912
C2	H19	0.0022575993133
C3	H19	0.0062706439982
O4	H19	0.0076340121943
C5	H19	0.00065449593698
H6	H19	9.2673254439e-05
H7	H19	2.4004178024e-05
C8	H19	0.00011511895717
H9	H19	4.9750990292e-05
N1	H19	5.4714156556e-06
C11	H19	1.3208663771e-05
O12	H19	6.651920248e-06
O13	H19	6.2880153791e-06
H14	H19	8.858479612e-07
H15	H19	0.00072092292382
H16	H19	0.00010907823958
H17	H19	0.00094383713538
O18	H19	0.47811276356

## ASPARAGINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.86645811184
C1	C3	0.041306176372
C2	C3	0.93245690465
C1	C4	0.0064621095204
C2	C4	0.031482529221
C3	C4	0.89261869458
C1	N5	0.0013776308527
C2	N5	0.008577352367
C3	N5	0.08629496378
C4	N5	0.88897856884
C1	O6	0.0023578170758
C2	O6	0.027859731248
C3	O6	0.10378088377
C4	O6	1.0985420268
N5	O6	0.26699533181
C1	O7	0.71474662463
C2	O7	0.077816542298
C3	O7	0.028034933927
C4	O7	0.0025448385901
N5	O7	0.00053349446799
O6	O7	0.0010720868353
C1	O8	1.1045959973
C2	O8	0.089983559037
C3	O8	0.011725326289
C4	O8	0.0019296507923
N5	O8	0.00056608851636
O6	O8	0.0011014829477
O7	O8	0.29366189027
C1	N9	0.054683361578
C2	N9	0.98215855774

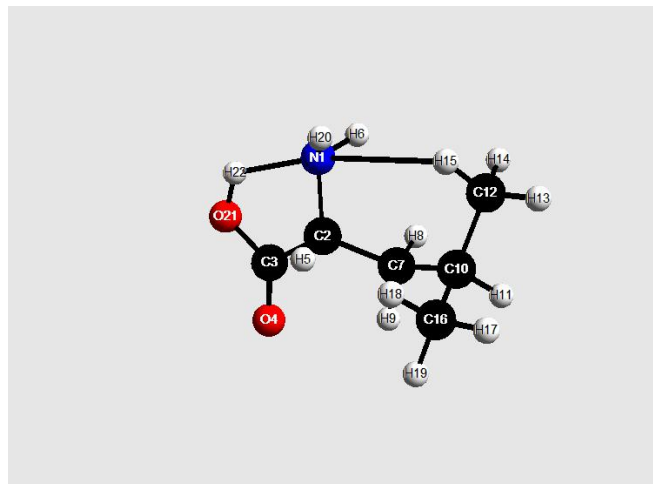
C3	N9	0.073256136217
C4	N9	0.010344359036
N5	N9	0.0023373324905
O6	N9	0.027331846835
O7	N9	0.010851635198
O8	N9	0.054201808586
C1	C1	0.046705537596
C2	C1	0.8978130422
C3	C1	0.036858882744
C4	C1	0.0032684621572
N5	C1	0.00097470793522
O6	C1	0.021475568389
O7	C1	0.012073005481
O8	C1	0.013788873402
N9	C1	0.064054180493
C1	H11	0.0042887557034
C2	H11	0.036610963216
C3	H11	0.94209985239
C4	H11	0.037599825428
N5	H11	0.016932828951
O6	H11	0.012994266928
O7	H11	0.0029156224526
O8	H11	0.0014555978172
N9	H11	0.015577720637
C1	H11	0.0094108072798
C1	H12	0.0024538739867
C2	H12	0.03319833884
C3	H12	0.93381043039
C4	H12	0.042758521495
N5	H12	0.012035264178
O6	H12	0.013787148323
O7	H12	0.024487333255
O8	H12	0.00079430553216
N9	H12	0.011154107745
C1	H12	0.0027638300009
H11	H12	0.036610489002
C1	H13	0.00026693766754
C2	H13	0.0013126781868
C3	H13	0.0076306968658
C4	H13	0.014837215843
N5	H13	0.798440024
O6	H13	0.011628739474
O7	H13	6.0482799296e-05
O8	H13	0.00012100787374
N9	H13	7.916441368e-05
C1	H13	4.3879470451e-05
H11	H13	0.00058270911734
H12	H13	0.00032042931352

C1	H14	4.3244572176e-05
C2	H14	0.00061499894912
C3	H14	0.0052619991347
C4	H14	0.014081024465
N5	H14	0.81528065262
O6	H14	0.01448745086
O7	H14	1.9138877029e-05
O8	H14	2.588560716e-05
N9	H14	0.00010829108975
C1	H14	0.00019729412713
H11	H14	0.0047431328108
H12	H14	0.000305072251
H13	H14	0.014659563123
C1	H15	0.0081695337311
C2	H15	0.0059118984442
C3	H15	0.0006020041538
C4	H15	3.4587365076e-05
N5	H15	1.3227927037e-05
O6	H15	4.7735273864e-05
O7	H15	0.54014527181
O8	H15	0.010555699906
N9	H15	0.001040810412
C1	H15	0.00019734611818
H11	H15	4.1802237167e-05
H12	H15	0.00051013007422
H13	H15	9.3896229523e-07
H14	H15	3.9435759598e-07
C1	H16	0.0060303868909
C2	H16	0.019897913805
C3	H16	0.0013671846817
C4	H16	0.0012468374898
N5	H16	0.00053047869531
O6	H16	0.016858133803
O7	H16	0.0012431457525
O8	H16	0.0024430712526
N9	H16	0.84153691504
C1	H16	0.0033167619323
H11	H16	0.00027263237062
H12	H16	0.00020359173418
H13	H16	1.0143309653e-05
H14	H16	4.6312855106e-05
H15	H16	0.0001794253456
C1	H17	0.003644637814
C2	H17	0.019398218066
C3	H17	0.0069449869126
C4	H17	0.00058912552051
N5	H17	0.00015171780344
O6	H17	0.0013641466669

O7	H17	0.00090732027586
O8	H17	0.026524766274
N9	H17	0.827181472
C1	H17	0.0010962986926
H11	H17	0.00031065335311
H12	H17	0.0014165876702
H13	H17	7.7165059416e-06
H14	H17	8.8406771524e-06
H15	H17	3.8492831903e-05
H16	H17	0.014152453065



# LEUCINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.93521753113
N1	C3	0.055931462508
C2	C3	0.85074720611
N1	O4	0.013701759666
C2	O4	0.10164441403
C3	O4	1.1010525884
N1	H5	0.060268345952
C2	H5	0.90494151932
C3	H5	0.043280169197
O4	H5	0.017337634915
N1	H6	0.85589092165
C2	H6	0.020141562885
C3	H6	0.0014564842468
O4	H6	0.00081088691253
H5	H6	0.0065360523144
N1	C7	0.064500445233
C2	C7	0.93894826192
C3	C7	0.036622007479
O4	C7	0.03163640449
H5	C7	0.03293329699
H6	C7	0.0079545631383
N1	H8	0.012935621781
C2	H8	0.04432404108
C3	H8	0.003368115679
O4	H8	0.0031237907094
H5	H8	0.0093825945668
H6	H8	0.0063670460212
C7	H8	0.94257799444
N1	H9	0.011523347415
C2	H9	0.037560870409

C3	H9	0.0049959816236
O4	H9	0.037163263859
H5	H9	0.0015306903694
H6	H9	0.00058277690654
C7	H9	0.92668145554
H8	H9	0.038478989298
N1	N1	0.0043183626459
C2	N1	0.036468258745
C3	N1	0.0071033248667
O4	N1	0.0028628411008
H5	N1	0.00501977066
H6	N1	0.00048950743482
C7	N1	0.95481570968
H8	N1	0.039930221908
H9	N1	0.036058951933
N1	H11	0.00068912312409
C2	H11	0.0093674635141
C3	H11	0.0011715647258
O4	H11	0.00027069464775
H5	H11	0.00050291007231
H6	H11	8.3467832679e-05
C7	H11	0.045987706561
H8	H11	0.0044498411655
H9	H11	0.005481927682
N1	H11	0.9334979696
N1	C12	0.015263553402
C2	C12	0.0033723903643
C3	C12	0.00026001191265
O4	C12	0.00061868397151
H5	C12	0.00038912130068
H6	C12	0.0033180104056
C7	C12	0.041320809269
H8	C12	0.007247342914
H9	C12	0.0083738425808
N1	C12	0.965581894
H11	C12	0.044612241223
N1	H13	0.0021437512483
C2	H13	0.00039680905835
C3	H13	0.00013554309125
O4	H13	0.0001608891371
H5	H13	5.2721731211e-05
H6	H13	0.00050488050518
C7	H13	0.009839456106
H8	H13	0.00062462839859
H9	H13	0.0015766715725
N1	H13	0.040129113811
H11	H13	0.0051816768221
C12	H13	0.96004263924

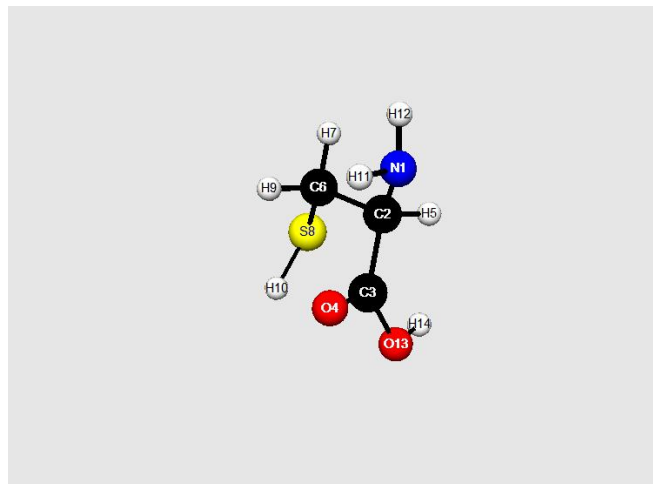
N1	H14	0.0039841115228
C2	H14	0.00048186323853
C3	H14	5.934980259e-05
O4	H14	5.1401968494e-05
H5	H14	0.00017406536382
H6	H14	0.003074176009
C7	H14	0.0076262121705
H8	H14	0.0068851334676
H9	H14	0.00060053317436
N1	H14	0.039707864142
H11	H14	0.003206600213
C12	H14	0.96042098124
H13	H14	0.043239145289
N1	H15	0.020544985186
C2	H15	0.001418563847
C3	H15	0.00018526963211
O4	H15	8.9505375712e-05
H5	H15	0.0003732030485
H6	H15	0.0011307212821
C7	H15	0.0026439450779
H8	H15	0.00036077685675
H9	H15	0.00037076823158
N1	H15	0.040020459942
H11	H15	0.011255588042
C12	H15	0.95381580474
H13	H15	0.043655758601
H14	H15	0.04447992057
N1	C16	0.00086974743577
C2	C16	0.0082753986452
C3	C16	0.00067916394899
O4	C16	0.00040617257326
H5	C16	0.011688617545
H6	C16	0.00026079560868
C7	C16	0.042683563918
H8	C16	0.0094208163288
H9	C16	0.0069920820372
N1	C16	0.96531197362
H11	C16	0.043742318387
C12	C16	0.047242385349
H13	C16	0.0073173426741
H14	C16	0.010267206958
H15	C16	0.0082242461025
N1	H17	0.00013447015194
C2	H17	0.001126368376
C3	H17	0.00011728046402
O4	H17	0.0001103556357
H5	H17	0.0017162400825
H6	H17	3.2807205788e-05

C7	H17	0.0097986894963
H8	H17	0.0019380855793
H9	H17	0.00059611779949
N1	H17	0.04039527667
H11	H17	0.0046683330848
C12	H17	0.0076685633222
H13	H17	0.00650138527
H14	H17	0.00079606105962
H15	H17	0.00056852767605
C16	H17	0.9608408562
N1	H18	0.00088814051203
C2	H18	0.007436951936
C3	H18	0.00069887707601
O4	H18	0.00028307182733
H5	H18	0.014881762173
H6	H18	8.6953417414e-05
C7	H18	0.0031838751478
H8	H18	0.00045581179381
H9	H18	0.00037598826968
N1	H18	0.040297599402
H11	H18	0.011224422396
C12	H18	0.0078159624029
H13	H18	0.00053145395393
H14	H18	0.00078554700352
H15	H18	0.0065704413024
C16	H18	0.95563984312
H17	H18	0.044251157633
N1	H19	0.00021769730909
C2	H19	0.00092790710089
C3	H19	0.00011047514808
O4	H19	0.00060371053099
H5	H19	0.0014649014969
H6	H19	3.4420942125e-05
C7	H19	0.0083555966104
H8	H19	0.00071781502836
H9	H19	0.0066517523077
N1	H19	0.039171832523
H11	H19	0.0032678197336
C12	H19	0.010099139679
H13	H19	0.00073693986545
H14	H19	0.0025055830651
H15	H19	0.00084558853144
C16	H19	0.95993803852
H17	H19	0.042401427496
H18	H19	0.043760831315
N1	C2	0.85551703177
C2	C2	0.019804126501
C3	C2	0.004821436804

O4	C2	0.0016146125679
H5	C2	0.0046327062773
H6	C2	0.016614551317
C7	C2	0.0018078350705
H8	C2	0.00045797020915
H9	C2	0.00049310264171
N1	C2	0.0003414173499
H11	C2	0.00017627337317
C12	C2	0.003616682296
H13	C2	0.0003561231604
H14	C2	0.00023900559307
H15	C2	0.0069070351581
C16	C2	0.00018008470695
H17	C2	3.0709382082e-05
H18	C2	0.00027460613093
H19	C2	2.7059696785e-05
N1	O21	0.090161836424
C2	O21	0.082281896601
C3	O21	0.74250601794
O4	O21	0.27897715733
H5	O21	0.0072496927467
H6	O21	0.0015760834709
C7	O21	0.0075186750393
H8	O21	0.00074644951129
H9	O21	0.0012174955695
N1	O21	0.0017606702135
H11	O21	0.00043323144107
C12	O21	0.00024420780699
H13	O21	5.3521494069e-05
H14	O21	4.4261984241e-05
H15	O21	0.00028156645906
C16	O21	0.00020146535571
H17	O21	3.8884187814e-05
H18	O21	0.00023084018856
H19	O21	6.8208928961e-05
C2	O21	0.0023253370554
N1	H22	0.054526252284
C2	H22	0.0023658494385
C3	H22	0.0063947349707
O4	H22	0.0072889295172
H5	H22	0.00014756741412
H6	H22	0.00078489538584
C7	H22	0.00056507585491
H8	H22	2.2958019019e-05
H9	H22	7.6907818448e-05
N1	H22	5.434436815e-05
H11	H22	1.6646074431e-05
C12	H22	7.4912047065e-05

H13	H22	2.1275009274e-05
H14	H22	1.3888459384e-05
H15	H22	0.00010386429019
C16	H22	7.6720436704e-06
H17	H22	7.9357685934e-07
H18	H22	4.8649922474e-06
H19	H22	2.1194581031e-06
C2	H22	0.00094686463119
O21	H22	0.46902937554

## CYSTEINE



## HARTREE-FOCK

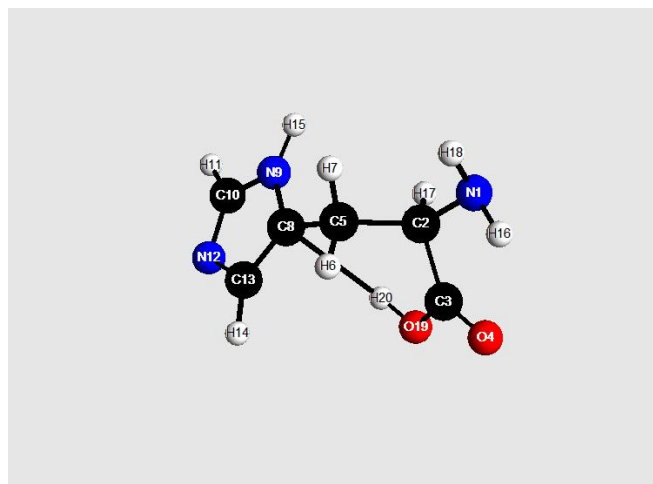
Atom A	Atom B	Delocalization index
N1	C2	0.97714207038
N1	C3	0.057959235788
C2	C3	0.85069856389
N1	O4	0.052599587318
C2	O4	0.096158426459
C3	O4	1.1118166768
N1	H5	0.060293585691
C2	H5	0.9098680374
C3	H5	0.03366663692
O4	H5	0.011077570912
N1	C6	0.081069577951
C2	C6	0.93381871006
C3	C6	0.04444323133
O4	C6	0.020505517683
H5	C6	0.040466822413
N1	H7	0.013248594609
C2	H7	0.036394279598
C3	H7	0.0082189605012
O4	H7	0.0032424419573
H5	H7	0.0033198049113
C6	H7	0.94761723683
N1	S8	0.023516960052
C2	S8	0.062358801149
C3	S8	0.0080182069115
O4	S8	0.003515438692
H5	S8	0.01878888703
C6	S8	1.0764749862
H7	S8	0.05415931686
N1	H9	0.010870073389
C2	H9	0.034430703235

C3	H9	0.0041318208281
O4	H9	0.010143784194
H5	H9	0.0093566935116
C6	H9	0.94325085739
H7	H9	0.034929952232
S8	H9	0.057622196043
N1	N1	0.00096098749667
C2	N1	0.0026505460346
C3	N1	0.0022373038628
O4	N1	0.0027300703344
H5	N1	0.0006465890791
C6	N1	0.044958706241
H7	N1	0.0096555039695
S8	N1	1.1236189343
H9	N1	0.0044654121147
N1	H11	0.82563058217
C2	H11	0.019957974316
C3	H11	0.0029162764338
O4	H11	0.021619911226
H5	H11	0.0083473625644
C6	H11	0.0025294802831
H7	H11	0.00025946502763
S8	H11	0.00071382675524
H9	H11	0.0013405280269
N1	H11	3.9731039352e-05
N1	H12	0.87201139986
C2	H12	0.021430248199
C3	H12	0.0073702115833
O4	H12	0.0031261095019
H5	H12	0.0011722856186
C6	H12	0.0063808235543
H7	H12	0.0044716412374
S8	H12	0.00075233009992
H9	H12	0.00035745206536
N1	H12	0.00012855603211
H11	H12	0.015761707277
N1	O13	0.010288382029
C2	O13	0.087630290235
C3	O13	0.72632184882
O4	O13	0.27807165131
H5	O13	0.020518242106
C6	O13	0.0086613717877
H7	O13	0.0013800599425
S8	O13	0.035338243343
H9	O13	0.00087074948409
N1	O13	0.010730098774
H11	O13	0.00084486645713
H12	O13	0.0017076581872



N1	H14	0.00060226930156
C2	H14	0.0042820843427
C3	H14	0.0069632858366
O4	H14	0.0097650353486
H5	H14	0.0046815871865
C6	H14	0.00048417991652
H7	H14	3.9900796502e-05
S8	H14	0.0089737860179
H9	H14	0.00023405976423
N1	H14	0.00035814216052
H11	H14	0.00012881574436
H12	H14	3.4727885263e-05
O13	H14	0.54350043213

# HISTIDINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.98197979328
N1	C3	0.052483351848
C2	C3	0.85739343921
N1	O4	0.061298038599
C2	O4	0.095981958999
C3	O4	1.1123594003
N1	C5	0.073705816932
C2	C5	0.91824123461
C3	C5	0.043240407012
O4	C5	0.014998867139
N1	H6	0.0073513263917
C2	H6	0.036095388409
C3	H6	0.0070163192824
O4	H6	0.0057028850863
C5	H6	0.9415237795
N1	H7	0.019229011679
C2	H7	0.037622945548
C3	H7	0.0077395115177
O4	H7	0.0027225985168
C5	H7	0.93608610515
H6	H7	0.038480784593
N1	C8	0.011542438208
C2	C8	0.041631019795
C3	C8	0.0027451736621
O4	C8	0.0012658247423
C5	C8	0.98643982612
H6	C8	0.043477782034
H7	C8	0.044389519902
N1	N9	0.0016232170251
C2	N9	0.0098762736674

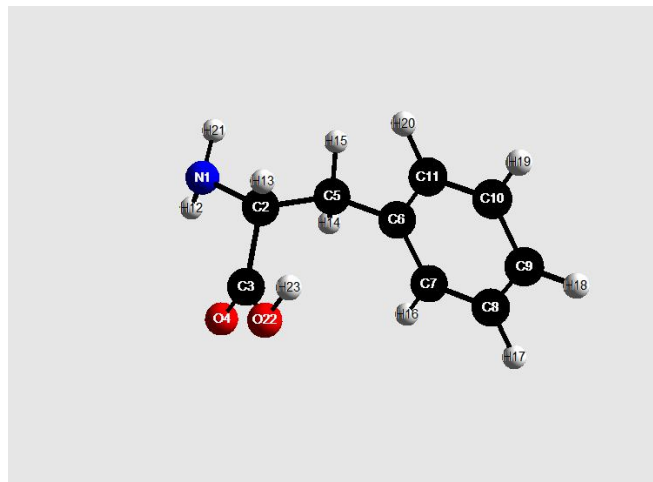
C3	N9	0.00079565579608
O4	N9	0.00054938333357
C5	N9	0.062744913319
H6	N9	0.0090583897236
H7	N9	0.011373144813
C8	N9	0.99217666061
N1	N1	0.0005747461902
C2	N1	0.0029713147212
C3	N1	0.00023248678539
O4	N1	0.0002221289242
C5	N1	0.0085035542805
H6	N1	0.0013142082253
H7	N1	0.002062226313
C8	N1	0.09208815923
N9	N1	0.9705376772
N1	H11	6.7623718963e-05
C2	H11	0.00027232320192
C3	H11	2.0475222928e-05
O4	H11	2.2913062104e-05
C5	H11	0.0013549695743
H6	H11	0.00040551469164
H7	H11	0.00022314383266
C8	H11	0.011617300906
N9	H11	0.064603379296
N1	H11	0.91744852482
N1	N12	0.00073287156958
C2	N12	0.0029794976531
C3	N12	0.00016201116736
O4	N12	0.00015884362747
C5	N12	0.012209879173
H6	N12	0.0010657155122
H7	N12	0.0031466630181
C8	N12	0.13593578876
N9	N12	0.25238767215
N1	N12	1.3275367753
H11	N12	0.068942785655
N1	C13	0.0022451065299
C2	C13	0.011785827244
C3	C13	0.00092997412312
O4	C13	0.00090831420318
C5	C13	0.042885492204
H6	C13	0.0080065273406
H7	C13	0.010733349964
C8	C13	1.4638225739
N9	C13	0.15613890863
N1	C13	0.056259473267
H11	C13	0.011403473558
N12	C13	1.1400648207

N1	H14	0.00010397721092
C2	H14	0.00058410624239
C3	H14	9.5277871067e-05
O4	H14	0.00011622395703
C5	H14	0.0033457183719
H6	H14	0.0025774754609
H7	H14	0.00051990566775
C8	H14	0.051491751916
N9	H14	0.013711505829
N1	H14	0.0076169811239
H11	H14	0.001321229344
N12	H14	0.054973616776
C13	H14	0.95450521235
N1	H15	0.00011671507279
C2	H15	0.00058973569003
C3	H15	5.9404396249e-05
O4	H15	5.6673991184e-05
C5	H15	0.0021378195153
H6	H15	0.00017312025494
H7	H15	0.0012476407587
C8	H15	0.015508163024
N9	H15	0.78536473286
N1	H15	0.013953111026
H11	H15	0.00098872442294
N12	H15	0.012368147136
C13	H15	0.0073153360027
H14	H15	0.0012388408538
N1	H16	0.80148455186
C2	H16	0.019071430361
C3	H16	0.0043187832921
O4	H16	0.034282972358
C5	H16	0.0018289752944
H6	H16	0.00031055468939
H7	H16	0.00047410586691
C8	H16	0.00044218922631
N9	H16	0.00017657707156
N1	H16	2.0118358525e-05
H11	H16	2.093881839e-06
N12	H16	4.5956826212e-05
C13	H16	9.946241482e-05
H14	H16	4.1421634426e-06
H15	H16	1.343991241e-05
N1	H17	0.063869740128
C2	H17	0.90913079013
C3	H17	0.039499709465
O4	H17	0.01221955888
C5	H17	0.039205897994
H6	H17	0.00919065352

H7	H17	0.0020601512983
C8	H17	0.008746824811
N9	H17	0.011727059439
N1	H17	0.00039214082104
H11	H17	3.3835825226e-05
N12	H17	0.0011300344078
C13	H17	0.00084220242601
H14	H17	7.1106448113e-05
H15	H17	0.0010372257856
H16	H17	0.0063332557399
N1	H18	0.87224939829
C2	H18	0.021503999958
C3	H18	0.0059398824452
O4	H18	0.0027309419976
C5	H18	0.0096481963185
H6	H18	0.00050815311583
H7	H18	0.0089214101074
C8	H18	0.0007384535411
N9	H18	0.00011316398317
N1	H18	0.00011049745388
H11	H18	9.2869802796e-06
N12	H18	0.00011535479109
C13	H18	0.00037433364861
H14	H18	1.6839198535e-05
H15	H18	8.3605699162e-06
H16	H18	0.014935117764
H17	H18	0.0013498636772
N1	O19	0.011779980917
C2	O19	0.088663708544
C3	O19	0.72512902727
O4	O19	0.27731836268
C5	O19	0.012404230921
H6	O19	0.0016793268233
H7	O19	0.0015539659122
C8	O19	0.025628412807
N9	O19	0.0025487009476
N1	O19	0.0020610536652
H11	O19	0.00016747318765
N12	O19	0.001794019161
C13	O19	0.019443279049
H14	O19	0.0028381820201
H15	O19	3.9054137984e-05
H16	O19	0.0011604886247
H17	O19	0.017027996996
H18	O19	0.0017701515003
N1	C2	0.00045439582928
C2	C2	0.0027296703901
C3	C2	0.0066517218726

O4	C2	0.0092193996375
C5	C2	0.0010650329715
H6	C2	5.5932315007e-05
H7	C2	0.00012175021384
C8	C2	0.014846942957
N9	C2	0.0022858587394
N1	C2	0.0011800427253
H11	C2	9.2100577857e-05
N12	C2	0.0013477507504
C13	C2	0.010873550634
H14	C2	0.00042593117499
H15	C2	1.7921219086e-05
H16	C2	7.5987990015e-05
H17	C2	0.0017207424454
H18	C2	3.5039730427e-05
O19	C2	0.52467838393

## PHENYLALANINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97670995531
N1	C3	0.057605224106
C2	C3	0.85350607666
N1	O4	0.05367328213
C2	O4	0.094997975739
C3	O4	1.1088387133
N1	C5	0.075998810224
C2	C5	0.92117569866
C3	C5	0.042971405018
O4	C5	0.018863623403
N1	C6	0.013264108638
C2	C6	0.042417366152
C3	C6	0.0053754012619
O4	C6	0.0016929970666
C5	C6	0.99020771164
N1	C7	0.0019532839021
C2	C7	0.0088196514406
C3	C7	0.0024280185172
O4	C7	0.0023955076319
C5	C7	0.048656519012
C6	C7	1.365019029
N1	C8	0.00039709603629
C2	C8	0.0012150064612
C3	C8	0.00024154600656
O4	C8	0.00030458546156
C5	C8	0.0077005337699
C6	C8	0.072197450886
C7	C8	1.3812775805
N1	C9	0.00075979674386
C2	C9	0.0036320530132

C3	C9	0.00029945479366
O4	C9	0.00014935448172
C5	C9	0.0047896618042
C6	C9	0.093455643819
C7	C9	0.073343517445
C8	C9	1.391342869
N1	N1	0.00030038024487
C2	N1	0.0011360948506
C3	N1	0.00027003592414
O4	N1	0.00021617953712
C5	N1	0.0079158640238
C6	N1	0.07117347854
C7	N1	0.097016508793
C8	N1	0.075490748545
C9	N1	1.3825661978
N1	C11	0.0020677418645
C2	C11	0.011406596947
C3	C11	0.00076847775323
O4	C11	0.00051674824866
C5	C11	0.048650881317
C6	C11	1.3560548369
C7	C11	0.072867895153
C8	C11	0.098212685982
C9	C11	0.073475666593
N1	C11	1.3934467518
N1	H12	0.82553726467
C2	H12	0.019855803212
C3	H12	0.0031842659616
O4	H12	0.023820036179
C5	H12	0.0022297861515
C6	H12	0.00032357359324
C7	H12	5.5535177603e-05
C8	H12	2.1523015447e-05
C9	H12	2.3688362031e-05
N1	H12	2.2749985947e-05
C11	H12	0.00015733139505
N1	H13	0.061801342494
C2	H13	0.91013416664
C3	H13	0.035249064257
O4	H13	0.01117857322
C5	H13	0.038575696877
C6	H13	0.0080129737041
C7	H13	0.00063212793529
C8	H13	0.00071979841623
C9	H13	0.00052328508822
N1	H13	0.0010416296999
C11	H13	0.0090429075517
H12	H13	0.0082487741432



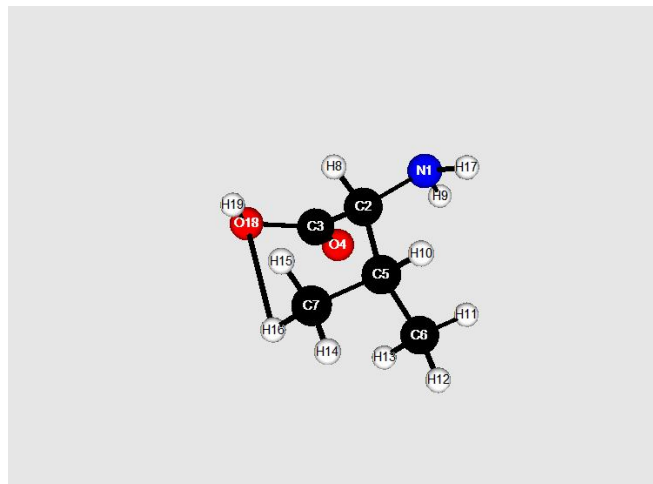
N1	H14	0.011232781197
C2	H14	0.037249605545
C3	H14	0.0048202417602
O4	H14	0.010262036025
C5	H14	0.93870091495
C6	H14	0.039407286749
C7	H14	0.011883374586
C8	H14	0.00095615846451
C9	H14	0.00079808508007
N1	H14	0.0014074114788
C11	H14	0.0073755150229
H12	H14	0.0012656086717
H13	H14	0.0095497519734
N1	H15	0.015276986793
C2	H15	0.039652797402
C3	H15	0.0083892018659
O4	H15	0.0032059945314
C5	H15	0.93972135364
C6	H15	0.042276293116
C7	H15	0.0085550295234
C8	H15	0.0014481047678
C9	H15	0.0021114324853
N1	H15	0.0010522840732
C11	H15	0.011744099568
H12	H15	0.00031298954188
H13	H15	0.0032362892185
H14	H15	0.038764763438
N1	H16	0.00016173418327
C2	H16	0.00060418982585
C3	H16	0.00080144916306
O4	H16	0.0032970676762
C5	H16	0.0097499775807
C6	H16	0.046562536297
C7	H16	0.96614457183
C8	H16	0.047626627745
C9	H16	0.0082037399047
N1	H16	0.005718764726
C11	H16	0.0083136161936
H12	H16	7.2843170883e-06
H13	H16	0.00012767463334
H14	H16	0.0082340174323
H15	H16	0.00078328264133
N1	H17	6.3171439856e-05
C2	H17	9.36158553e-05
C3	H17	9.0398393646e-06
O4	H17	1.5460126209e-05
C5	H17	0.0011227560491
C6	H17	0.0083989486139

C7	H17	0.048539457405
C8	H17	0.97470214823
C9	H17	0.048671890938
N1	H17	0.0085953886059
C11	H17	0.0060063387334
H12	H17	2.1959552435e-06
H13	H17	4.3196001837e-05
H14	H17	6.1584667345e-05
H15	H17	0.00021057529798
H16	H17	0.0056836536365
N1	H18	5.3562317828e-05
C2	H18	0.00024500947341
C3	H18	2.1152440346e-05
O4	H18	1.7811909815e-05
C5	H18	0.00035958334545
C6	H18	0.0058062666828
C7	H18	0.0085430056594
C8	H18	0.048988222298
C9	H18	0.97656773265
N1	H18	0.048894073043
C11	H18	0.0085657082187
H12	H18	1.5906881375e-06
H13	H18	4.3573800929e-05
H14	H18	7.9383431637e-05
H15	H18	0.00016323203042
H16	H18	0.001293193102
H17	H18	0.0055560968242
N1	H19	4.5338072772e-05
C2	H19	6.2556874434e-05
C3	H19	1.569090816e-05
O4	H19	1.5778340985e-05
C5	H19	0.0011565258501
C6	H19	0.0085403365262
C7	H19	0.0060932084124
C8	H19	0.008582313037
C9	H19	0.048525644516
N1	H19	0.9760978972
C11	H19	0.049595822703
H12	H19	2.0502377593e-06
H13	H19	3.5997326562e-05
H14	H19	0.00025906873638
H15	H19	5.6093839714e-05
H16	H19	0.00037519266077
H17	H19	0.0013927178222
H18	H19	0.0055257548929
N1	C2	0.00039272723676
C2	C2	0.0024022734295
C3	C2	0.00020935823186

O4	C2	0.00017293671782
C5	C2	0.0094117936279
C6	C2	0.04712470433
C7	C2	0.0084793251705
C8	C2	0.0061441637617
C9	C2	0.0084713912908
N1	C2	0.049818423002
C11	C2	0.97127586815
H12	C2	6.2305797257e-05
H13	C2	0.0042642487679
H14	C2	0.00077197525065
H15	C2	0.0060314924058
H16	C2	0.0015621184666
H17	C2	0.00039091842526
H18	C2	0.0013403070484
H19	C2	0.0058647759157
N1	H21	0.8745338208
C2	H21	0.021427617135
C3	H21	0.0072916428316
O4	H21	0.0030768849017
C5	H21	0.0070080785118
C6	H21	0.00054597150326
C7	H21	0.00019805307657
C8	H21	3.3601327925e-05
C9	H21	8.1824852374e-05
N1	H21	1.6465615208e-05
C11	H21	0.00014247235108
H12	H21	0.015789022626
H13	H21	0.0010872504839
H14	H21	0.00042857813066
H15	H21	0.0058230447232
H16	H21	9.5706707486e-06
H17	H21	5.3091063604e-06
H18	H21	5.5228838483e-06
H19	H21	1.2621052841e-06
C2	H21	2.2910474581e-05
N1	O22	0.010575760818
C2	O22	0.087746488459
C3	O22	0.72436576489
O4	O22	0.27715554223
C5	O22	0.0082716445247
C6	O22	0.019064950348
C7	O22	0.016478296007
C8	O22	0.0027198307179
C9	O22	0.001230664916
N1	O22	0.0012168210553
C11	O22	0.0043788112571
H12	O22	0.00090684747504

H13	O22	0.021107955578
H14	O22	0.00083413482969
H15	O22	0.0013343973321
H16	O22	0.0013704616278
H17	O22	8.8656822247e-05
H18	O22	7.2474566386e-05
H19	O22	6.3869853097e-05
C2	O22	0.00013388926398
H21	O22	0.0017428697746
N1	H23	0.00062272242196
C2	H23	0.0041265317083
C3	H23	0.0070176584344
O4	H23	0.0098934026518
C5	H23	0.0003475251301
C6	H23	0.0032538250816
C7	H23	0.00060504910826
C8	H23	0.00027886353265
C9	H23	0.00025008440151
N1	H23	0.00064046322394
C11	H23	0.0031627848254
H12	H23	0.00012963084956
H13	H23	0.0045269900892
H14	H23	0.00012869559122
H15	H23	3.3721891911e-05
H16	H23	1.7084835024e-05
H17	H23	1.5464427802e-05
H18	H23	1.3999684323e-05
H19	H23	1.7865364486e-05
C2	H23	0.0001298421474
H21	H23	3.516312096e-05
O22	H23	0.54803661174

## VALINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97423803026
N1	C3	0.058324909559
C2	C3	0.85664400864
N1	O4	0.052850120752
C2	O4	0.092795403482
C3	O4	1.1138057421
N1	C5	0.067005605872
C2	C5	0.91602044726
C3	C5	0.040314793829
O4	C5	0.01336779309
N1	C6	0.016131912537
C2	C6	0.037177412739
C3	C6	0.0055308028565
O4	C6	0.015441790518
C5	C6	0.96793513561
N1	C7	0.011462929014
C2	C7	0.041521779533
C3	C7	0.0041886489152
O4	C7	0.00099816045598
C5	C7	0.96763199379
C6	C7	0.045725920919
N1	H8	0.063855619125
C2	H8	0.90719823085
C3	H8	0.037418107225
O4	H8	0.01152402276
C5	H8	0.038079353191
C6	H8	0.0084481068741
C7	H8	0.0098121533591
N1	H9	0.8217122862
C2	H9	0.019478260443

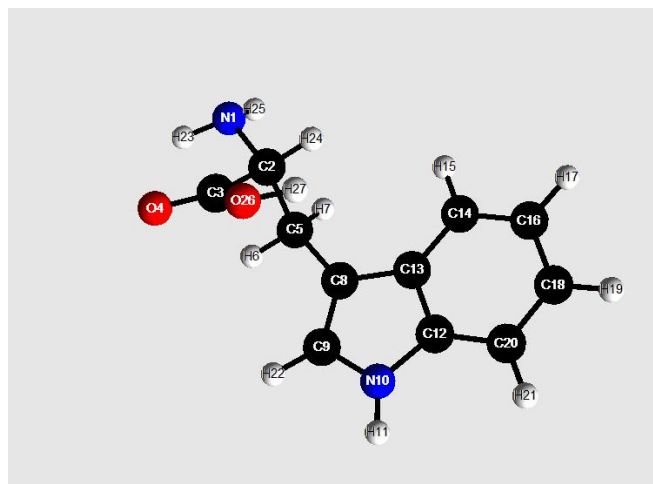
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O4	H9	0.024235114321
C5	H9	0.0015030047989
C6	H9	0.0022989773265
C7	H9	0.00043304474677
H8	H9	0.0078858776178
N1	N1	0.014135207397
C2	N1	0.043484883463
C3	N1	0.0084026533328
O4	N1	0.0026981398312
C5	N1	0.93034180816
C6	N1	0.042184839604
C7	N1	0.043244812344
H8	N1	0.0042018399497
H9	N1	0.0003428020626
N1	H11	0.02138003543
C2	H11	0.0036653715712
C3	H11	0.00036250970374
O4	H11	0.002738655017
C5	H11	0.039823201565
C6	H11	0.95651254644
C7	H11	0.0099578889207
H8	H11	0.00047655279043
H9	H11	0.0041099388752
N1	H11	0.00329399195
N1	H12	0.0016527964302
C2	H12	0.009776992905
C3	H12	0.00085669776508
O4	H12	0.0019286581583
C5	H12	0.042141727563
C6	H12	0.96110882338
C7	H12	0.0081712974983
H8	H12	0.0016843427534
H9	H12	0.00035090697127
N1	H12	0.0043453660641
H11	H12	0.042320882611
N1	H13	0.00081456720436
C2	H13	0.0030798847876
C3	H13	0.0032534675692
O4	H13	0.019722196105
C5	H13	0.03987915183
C6	H13	0.95128450456
C7	H13	0.0073345105335
H8	H13	0.00032289418764
H9	H13	0.00010217421124
N1	H13	0.010993473985
H11	H13	0.041126592082
H12	H13	0.041483188763

N1	H14	0.0024872336859
C2	H14	0.0094913037185
C3	H14	0.00056406794523
O4	H14	0.00022916318441
C5	H14	0.040005160916
C6	H14	0.0076916461577
C7	H14	0.95928398201
H8	H14	0.00093087914094
H9	H14	7.0085703515e-05
N1	H14	0.0045248001385
H11	H14	0.00076282135597
H12	H14	0.0069540817044
H13	H14	0.00050421091126
N1	H15	0.0010852685922
C2	H15	0.0078543690265
C3	H15	0.00046767840893
O4	H15	0.00033837670829
C5	H15	0.040736297385
C6	H15	0.010122536998
C7	H15	0.96158503311
H8	H15	0.0096659358417
H9	H15	0.00017805562496
N1	H15	0.0034565541093
H11	H15	0.0025366076521
H12	H15	0.00080230049036
H13	H15	0.00073634724589
H14	H15	0.043213726136
N1	H16	0.00058881110226
C2	H16	0.003056274397
C3	H16	0.002083378479
O4	H16	0.00094486142013
C5	H16	0.039577782554
C6	H16	0.007603380374
C7	H16	0.95282132987
H8	H16	0.00044099852741
H9	H16	2.5522506258e-05
N1	H16	0.010984569688
H11	H16	0.00075279751919
H12	H16	0.00053536048576
H13	H16	0.0057408523274
H14	H16	0.041608655581
H15	H16	0.04335783171
N1	H17	0.87353513403
C2	H17	0.021298712895
C3	H17	0.0071577813824
O4	H17	0.0029123625989
C5	H17	0.0071448446593
C6	H17	0.00097181421489

C7	H17	0.00053276632612
H8	H17	0.0010383869024
H9	H17	0.015711937229
N1	H17	0.0062217424546
H11	H17	0.0014599591354
H12	H17	0.00012211820904
H13	H17	0.00015072239807
H14	H17	7.5448894175e-05
H15	H17	3.2799787777e-05
H16	H17	0.00019599756918
N1	O18	0.010960780923
C2	O18	0.087273172385
C3	O18	0.71761277717
O4	O18	0.27684995549
C5	O18	0.0077122257099
C6	O18	0.00091438154657
C7	O18	0.016176561983
H8	O18	0.022107802293
H9	O18	0.00090708625843
N1	O18	0.0013794958712
H11	O18	0.00013525630054
H12	O18	0.00026214390185
H13	O18	0.00073249727329
H14	O18	0.0022329765597
H15	O18	0.0033582865712
H16	O18	0.020554879374
H17	O18	0.001776764712
N1	H19	0.00072749182273
C2	H19	0.0044655869218
C3	H19	0.0071127322979
O4	H19	0.010177984605
C5	H19	0.00038909016349
C6	H19	0.00019044299097
C7	H19	0.0024145914208
H8	H19	0.0053124810311
H9	H19	0.00014616599719
N1	H19	4.3929243501e-05
H11	H19	1.9343383359e-05
H12	H19	2.1537244975e-05
H13	H19	1.5293305013e-05
H14	H19	0.000447841088
H15	H19	0.0020350784588
H16	H19	0.00072409872163
H17	H19	3.5980898811e-05
O18	H19	0.55786377916



## TRYPTOPHAN



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97332966826
N1	C3	0.058596324953
C2	C3	0.85296677302
N1	O4	0.05136970983
C2	O4	0.094496397462
C3	O4	1.1061329087
N1	C5	0.075268166865
C2	C5	0.92085992626
C3	C5	0.042715316024
O4	C5	0.019878933822
N1	H6	0.011842777192
C2	H6	0.037478981311
C3	H6	0.0046012117002
O4	H6	0.011556037379
C5	H6	0.9387452811
N1	H7	0.014407764835
C2	H7	0.040115051634
C3	H7	0.0083894549039
O4	H7	0.0032994689105
C5	H7	0.93862247336
H6	H7	0.039094443383
N1	C8	0.013021315997
C2	C8	0.043446937897
C3	C8	0.0077264128372
O4	C8	0.0031257112428
C5	C8	1.0043343945
H6	C8	0.042112971814
H7	C8	0.043674087579
N1	C9	0.0027559452477
C2	C9	0.012987434168

C3	C9	0.0028639336756
O4	C9	0.0029113353938
C5	C9	0.053856673905
H6	C9	0.0105875375
H7	C9	0.012027067584
C8	C9	1.5223184238
N1	N1	0.0009487105987
C2	N1	0.0038270884915
C3	N1	0.00041456500855
O4	N1	0.00028226443714
C5	N1	0.012453378093
H6	N1	0.0011049187067
H7	N1	0.003378355643
C8	N1	0.15998272417
C9	N1	1.0057827631
N1	H11	7.2646604876e-05
C2	H11	0.00015953201209
C3	H11	9.8502685614e-06
O4	H11	6.1335760283e-06
C5	H11	0.0010365298692
H6	H11	3.5479640909e-05
H7	H11	0.00019604781465
C8	H11	0.0072803550058
C9	H11	0.015821211895
N1	H11	0.79022301853
N1	C12	0.00023228071144
C2	C12	0.00075142534299
C3	C12	0.00020689326359
O4	C12	0.00022548557735
C5	C12	0.0067383528965
H6	C12	0.0011816785676
H7	C12	0.00056952948904
C8	C12	0.06265248567
C9	C12	0.06907258291
N1	C12	0.98608460336
H11	C12	0.016037702661
N1	C13	0.0011013600392
C2	C13	0.0060029686169
C3	C13	0.00051832492639
O4	C13	0.00043300994823
C5	C13	0.036662285585
H6	C13	0.0075364647812
H7	C13	0.0058498792391
C8	C13	1.1413389094
C9	C13	0.080183651998
N1	C13	0.12715230879
H11	C13	0.0073379154183
C12	C13	1.2338541718

N1	C14	0.0003768532482
C2	C14	0.0025640700055
C3	C14	0.00026966694151
O4	C14	0.00021859492646
C5	C14	0.0047213834721
H6	C14	0.00051830878535
H7	C14	0.0036998436223
C8	C14	0.044640439488
C9	C14	0.025798880768
N1	C14	0.013471314613
H11	C14	0.0011264129846
C12	C14	0.065337972531
C13	C14	1.2949194577
N1	H15	0.00035176391147
C2	H15	0.0029525359838
C3	H15	0.00026007232568
O4	H15	0.00021110254705
C5	H15	0.0035232016707
H6	H15	0.00045967933718
H7	H15	0.0041284093771
C8	H15	0.0041665043839
C9	H15	0.0011686073443
N1	H15	0.0017558115851
H11	H15	0.0003037585656
C12	H15	0.0081059954647
C13	H15	0.04502450813
C14	H15	0.97266481061
N1	C16	8.3101837283e-05
C2	C16	0.00043733840905
C3	C16	4.3126194122e-05
O4	C16	3.7013728797e-05
C5	C16	0.00064204844289
H6	C16	0.00010207112796
H7	C16	0.00057963311934
C8	C16	0.01612658199
C9	C16	0.007793148952
N1	C16	0.019258616788
H11	C16	0.00050965989616
C12	C16	0.072921689222
C13	C16	0.071307325134
C14	C16	1.4567165703
H15	C16	0.051104294411
N1	H17	7.2441633076e-06
C2	H17	2.4251108158e-05
C3	H17	2.1459868211e-06
O4	H17	3.0780894697e-06
C5	H17	3.9314491769e-05
H6	H17	1.5891319415e-05

H7	H17	2.8293135295e-05
C8	H17	0.0017641778214
C9	H17	0.00066164685599
N1	H17	0.001480365048
H11	H17	4.6291982693e-05
C12	H17	0.0048505070389
C13	H17	0.0091421982739
C14	H17	0.053180191266
H15	H17	0.0060590291085
C16	H17	0.97882992124
N1	C18	4.6452105037e-05
C2	C18	0.0002649771703
C3	C18	9.0321286244e-05
O4	C18	9.7441523536e-05
C5	C18	0.00058046812012
H6	C18	0.00015276597899
H7	C18	0.00029183492772
C8	C18	0.0076514726858
C9	C18	0.021929703524
N1	C18	0.019168939023
H11	C18	0.00030920805442
C12	C18	0.073732311945
C13	C18	0.075204115094
C14	C18	0.073585572999
H15	C18	0.0087750865863
C16	C18	1.3155007996
H17	C18	0.047400456461
N1	H19	4.98658853e-06
C2	H19	2.5949374974e-05
C3	H19	6.891124967e-06
O4	H19	7.2982405586e-06
C5	H19	4.8527604665e-05
H6	H19	1.2439698637e-05
H7	H19	3.4166250835e-05
C8	H19	0.00056951899145
C9	H19	0.0017537196881
N1	H19	0.0019846834922
H11	H19	1.7534334032e-05
C12	H19	0.0088756886227
C13	H19	0.0048782916662
C14	H19	0.00837949062
H15	H19	0.0012933697067
C16	H19	0.046327481269
H17	H19	0.0054916005925
C18	H19	0.97657663578
N1	C2	5.3450219213e-05
C2	C2	0.00018957674277
C3	C2	3.2909647333e-05

O4	C2	3.1772882355e-05
C5	C2	0.0010092686273
H6	C2	0.00024605945713
H7	C2	0.00021769016245
C8	C2	0.0077315510605
C9	C2	0.014387362876
N1	C2	0.086741412
H11	C2	0.0024440476542
C12	C2	1.2747044997
C13	C2	0.056449669363
C14	C2	0.093202958461
H15	C2	0.0058390472937
C16	C2	0.071832270707
H17	C2	0.0085064826753
C18	C2	1.4515627807
H19	C2	0.052662951131
N1	H21	1.3682230915e-05
C2	H21	2.2020232527e-05
C3	H21	2.7440539774e-06
O4	H21	3.2876874683e-06
C5	H21	0.00033724732219
H6	H21	6.5363884711e-05
H7	H21	2.2500160904e-05
C8	H21	0.0013445607445
C9	H21	0.00050014851878
N1	H21	0.008258411547
H11	H21	0.0012430621854
C12	H21	0.0470234815
C13	H21	0.0075289208757
C14	H21	0.0058153061306
H15	H21	0.0004221283014
C16	H21	0.0087854806075
H17	H21	0.0012851783442
C18	H21	0.049738260484
H19	H21	0.0059783293842
C2	H21	0.97665436702
N1	H22	0.0001458327061
C2	H22	0.00065293037872
C3	H22	0.00028059761755
O4	H22	0.001462364971
C5	H22	0.0048712301764
H6	H22	0.0037734888712
H7	H22	0.00060638642923
C8	H22	0.045984412695
C9	H22	0.9497298324
N1	H22	0.061006348347
H11	H22	0.0013899285828
C12	H22	0.0090068378009

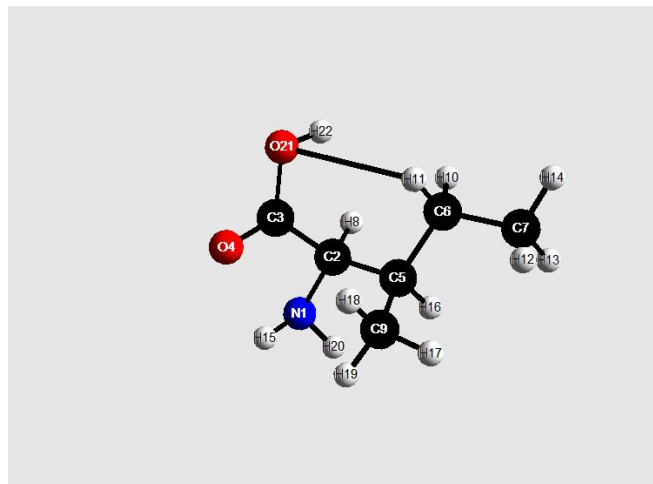
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H17	H22	0.0001072129742
C18	H22	0.001796112858
H19	H22	0.00017435639071
C2	H22	0.0016503775773
H21	H22	3.5524254334e-05
N1	H23	0.83053985283
C2	H23	0.019943151347
C3	H23	0.0030672584428
O4	H23	0.022151335321
C5	H23	0.002398491526
H6	H23	0.0015175426305
H7	H23	0.00029721321408
C8	H23	0.00030385416799
C9	H23	7.1956817309e-05
N1	H23	2.426258326e-05
H11	H23	1.6264761021e-06
C12	H23	1.4520284947e-05
C13	H23	0.00011033358522
C14	H23	8.1761830092e-05
H15	H23	7.6095533418e-05
C16	H23	8.1053163546e-06
H17	H23	4.7188924883e-07
C18	H23	7.7635843027e-06
H19	H23	7.5332145265e-07
C2	H23	5.8592832792e-06
H21	H23	7.9210379693e-07
H22	H23	5.1745893541e-06
N1	H24	0.061697980184
C2	H24	0.90943866827
C3	H24	0.035124195749
O4	H24	0.010936544284
C5	H24	0.037875641177
H6	H24	0.0095759866625
H7	H24	0.0032065207554
C8	H24	0.0059540993999
C9	H24	0.00058857649555
N1	H24	0.0004033282709
H11	H24	1.5186338977e-05
C12	H24	0.00040404523808
C13	H24	0.0055111354971
C14	H24	0.0076364514037
H15	H24	0.0061673073294
C16	H24	0.00090121713994
H17	H24	3.2134631064e-05

C18	H24	0.00038580006794
H19	H24	4.0340639045e-05
C2	H24	0.00039234348738
H21	H24	2.4882889668e-05
H22	H24	9.0039415429e-05
H23	H24	0.0083805026334
N1	H25	0.87586792227
C2	H25	0.021365730835
C3	H25	0.0074204594586
O4	H25	0.0030820999562
C5	H25	0.0066296595884
H6	H25	0.00042723637956
H7	H25	0.0054695226682
C8	H25	0.00056922476547
C9	H25	0.00029635345673
N1	H25	0.00010400605503
H11	H25	4.8706269104e-06
C12	H25	1.5076746786e-05
C13	H25	5.8021629367e-05
C14	H25	2.5729011472e-05
H15	H25	3.1576471477e-05
C16	H25	1.0791021018e-05
H17	H25	7.630645958e-07
C18	H25	7.4755583858e-06
H19	H25	7.7592287249e-07
C2	H25	5.4291224045e-06
H21	H25	6.3203031795e-07
H22	H25	1.1329183637e-05
H23	H25	0.015998658258
H24	H25	0.0011394311602
N1	O26	0.01041028393
C2	O26	0.087090363861
C3	O26	0.72423598201
O4	O26	0.27715013677
C5	O26	0.0080871080632
H6	O26	0.00087832871795
H7	O26	0.0014090818263
C8	O26	0.021785410053
C9	O26	0.012171646175
N1	O26	0.0019927346775
H11	O26	3.8355432509e-05
C12	O26	0.00093190892827
C13	O26	0.0049535364578
C14	O26	0.00068342374615
H15	O26	6.4247070642e-05
C16	O26	0.00017450688507
H17	O26	1.3929822423e-05
C18	O26	0.00026355079568

H19	O26	1.8461434321e-05
C2	O26	0.0001031206266
H21	O26	6.1693626947e-06
H22	O26	0.00055055157998
H23	O26	0.00087167369356
H24	O26	0.02160431638
H25	O26	0.0017097314314
N1	H27	0.00060276366043
C2	H27	0.0042157900794
C3	H27	0.0070208907752
O4	H27	0.0098495168976
C5	H27	0.00029090668795
H6	H27	0.00012272101035
H7	H27	3.1513817616e-05
C8	H27	0.0019248995829
C9	H27	0.00027279683121
N1	H27	0.00034034470066
H11	H27	8.9374015478e-06
C12	H27	0.00047769124319
C13	H27	0.0030934611624
C14	H27	0.0010098265822
H15	H27	5.1030694934e-05
C16	H27	0.00012511767858
H17	H27	5.4674541025e-06
C18	H27	0.00019463318666
H19	H27	1.1372327319e-05
C2	H27	8.1949786341e-05
H21	H27	4.1262637096e-06
H22	H27	8.7681270547e-06
H23	H27	0.00013223011091
H24	H27	0.0047950961495
H25	H27	3.3608797121e-05
O26	H27	0.54749356245



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### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97370540456
N1	C3	0.058347895861
C2	C3	0.85710837846
N1	O4	0.053339923208
C2	O4	0.092607418507
C3	O4	1.1135503338
N1	C5	0.066622557842
C2	C5	0.91456578424
C3	C5	0.040255646237
O4	C5	0.013225148807
N1	C6	0.010988714686
C2	C6	0.040286370108
C3	C6	0.0037451170548
O4	C6	0.00087584482662
C5	C6	0.95608572124
N1	C7	0.0020203012745
C2	C7	0.0081079266873
C3	C7	0.00054851228948
O4	C7	0.00022580151896
C5	C7	0.039754009961
C6	C7	0.97601897357
N1	H8	0.063844721819
C2	H8	0.90577522003
C3	H8	0.037563394725
O4	H8	0.011526923007
C5	H8	0.037529066488
C6	H8	0.010241116727
C7	H8	0.00090248111297
N1	C9	0.016382453529
C2	C9	0.037745251287

C3	C9	0.0058946334668
O4	C9	0.015812151808
C5	C9	0.96794398093
C6	C9	0.041006102278
C7	C9	0.0085383832755
H8	C9	0.0083574700045
N1	N1	0.0012949227958
C2	N1	0.010569216136
C3	N1	0.00057412951269
O4	N1	0.00041985459903
C5	N1	0.041478631025
C6	N1	0.94330594661
C7	N1	0.044191484176
H8	N1	0.013188361893
C9	N1	0.009392514809
N1	H11	0.00053567410956
C2	H11	0.0027531105109
C3	H11	0.0020333150713
O4	H11	0.00085582521521
C5	H11	0.039921038928
C6	H11	0.93977738954
C7	H11	0.041548953832
H8	H11	0.00052865751838
C9	H11	0.0079995234604
N1	H11	0.043276535644
N1	H12	0.00013078561143
C2	H12	0.00047180887897
C3	H12	2.9043389183e-05
O4	H12	3.6723813365e-05
C5	H12	0.0030432456438
C6	H12	0.040588288841
C7	H12	0.95795632945
H8	H12	0.00031265639535
C9	H12	0.0094622543443
N1	H12	0.011114558084
H11	H12	0.0038132191397
N1	H13	8.5418087055e-05
C2	H13	0.00060602595534
C3	H13	0.00019621703688
O4	H13	7.5216959132e-05
C5	H13	0.0074131014518
C6	H13	0.042050589855
C7	H13	0.96172703923
H8	H13	4.8808649131e-05
C9	H13	0.00077709545106
N1	H13	0.0033901557887
H11	H13	0.010920450778
H12	H13	0.043762003002

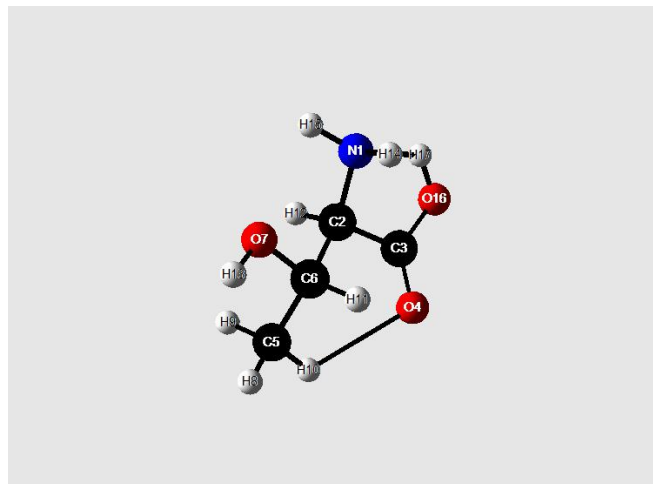
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C2	H14	0.0014849453537
C3	H14	5.947167406e-05
O4	H14	4.97243895e-05
C5	H14	0.0098957677992
C6	H14	0.042933222806
C7	H14	0.9648306237
H8	H14	4.3395302668e-05
C9	H14	0.0010498388907
N1	H14	0.0048835993078
H11	H14	0.0034448488378
H12	H14	0.042807411465
H13	H14	0.043641029029
N1	H15	0.82057191513
C2	H15	0.019408195974
C3	H15	0.0034879016568
O4	H15	0.02485780117
C5	H15	0.0014762373143
C6	H15	0.00043811801268
C7	H15	6.3482604449e-05
H8	H15	0.0077510599869
C9	H15	0.0022970030223
N1	H15	0.000219632952
H11	H15	2.7812139268e-05
H12	H15	1.3996601404e-05
H13	H15	3.766672733e-06
H14	H15	1.2777824909e-05
N1	H16	0.014651961449
C2	H16	0.043116922865
C3	H16	0.008238514172
O4	H16	0.0026234594551
C5	H16	0.92622605138
C6	H16	0.040635858169
C7	H16	0.0094032679027
H8	H16	0.0039876841248
C9	H16	0.042092097778
N1	H16	0.002942663715
H11	H16	0.010420669016
H12	H16	0.00044032915721
H13	H16	0.0080087928019
H14	H16	0.00091299047516
H15	H16	0.0003566459388
N1	H17	0.0015432923163
C2	H17	0.0095860401488
C3	H17	0.00088564174104
O4	H17	0.0019674808935
C5	H17	0.041058267132
C6	H17	0.0035636783117

C7	H17	0.010464453489
H8	H17	0.0016950621808
C9	H17	0.9569618498
N1	H17	0.00038656001754
H11	H17	0.00039053678698
H12	H17	0.014887253813
H13	H17	0.00098183623317
H14	H17	0.0014212503251
H15	H17	0.00032060450518
H16	H17	0.0045479051163
N1	H18	0.00090530799615
C2	H18	0.0029015997232
C3	H18	0.0032609005332
O4	H18	0.018115740087
C5	H18	0.039974639662
C6	H18	0.0073685454617
C7	H18	0.00070926995712
H8	H18	0.00032376959319
C9	H18	0.95159639706
N1	H18	0.00067590573067
H11	H18	0.0064357984277
H12	H18	0.00083302942208
H13	H18	0.00022147144954
H14	H18	6.1373224776e-05
H15	H18	9.8387726387e-05
H16	H18	0.01091345696
H17	H18	0.04144645415
N1	H19	0.022998131702
C2	H19	0.0043137132146
C3	H19	0.0004450100361
O4	H19	0.0038031415244
C5	H19	0.039728348739
C6	H19	0.0095375743549
C7	H19	0.00096487829329
H8	H19	0.00050692911983
C9	H19	0.95424093803
N1	H19	0.0021214559651
H11	H19	0.00074749657131
H12	H19	0.0012478260392
H13	H19	7.1382972453e-05
H14	H19	0.00012007111873
H15	H19	0.0044502452956
H16	H19	0.0029196714548
H17	H19	0.041748819395
H18	H19	0.041089875325
N1	C2	0.87345811133
C2	C2	0.021282307506
C3	C2	0.0071141108265

O4	C2	0.002908831651
C5	C2	0.0073253742474
C6	C2	0.00053358819593
C7	C2	7.2800989745e-05
H8	C2	0.0010359719798
C9	C2	0.0009590149268
N1	C2	3.7628521444e-05
H11	C2	0.00019108848365
H12	C2	4.6560875127e-06
H13	C2	1.7684167771e-05
H14	C2	1.5843705493e-05
H15	C2	0.015682922884
H16	C2	0.0065015823768
H17	C2	0.00011862606261
H18	C2	0.00015463934377
H19	C2	0.0014662944619
N1	O21	0.011034796089
C2	O21	0.087113704326
C3	O21	0.71753360039
O4	O21	0.27675912365
C5	O21	0.0076962887151
C6	O21	0.015511391156
C7	O21	0.0020451422253
H8	O21	0.021750871344
C9	O21	0.00095769172638
N1	O21	0.0048621190661
H11	O21	0.021054275391
H12	O21	0.00012254300263
H13	O21	0.00049266971852
H14	O21	6.9253445855e-05
H15	O21	0.00091818425669
H16	O21	0.0013359552339
H17	O21	0.00025061704133
H18	O21	0.00078345864666
H19	O21	0.00017111824574
C2	O21	0.0017832986175
N1	H22	0.00069906284509
C2	H22	0.0042954252264
C3	H22	0.0070883581819
O4	H22	0.010145455599
C5	H22	0.00044635808335
C6	H22	0.0028146331408
C7	H22	0.00046187573216
H8	H22	0.0050843816347
C9	H22	0.00020967539851
N1	H22	0.0029840013609
H11	H22	0.00080314221707
H12	H22	0.000110868701

H13	H22	2.5493843088e-05
H14	H22	1.6740590567e-05
H15	H22	0.00013863484817
H16	H22	4.3295944823e-05
H17	H22	2.3026659676e-05
H18	H22	1.4405390608e-05
H19	H22	2.1578974227e-05
C2	H22	3.604596144e-05
O21	H22	0.55674217172

## THREONINE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.95848750317
N1	C3	0.056513113381
C2	C3	0.85654309592
N1	O4	0.014117788972
C2	O4	0.099735381095
C3	O4	1.1078884774
N1	C5	0.0095254015508
C2	C5	0.037087747261
C3	C5	0.0021019391103
O4	C5	0.02363655247
N1	C6	0.059028763827
C2	C6	0.89768084509
C3	C6	0.031084150487
O4	C6	0.020871489228
C5	C6	0.94261374792
N1	O7	0.0565298569
C2	O7	0.076685026399
C3	O7	0.0075580011321
O4	O7	0.0029055073975
C5	O7	0.091597576034
C6	O7	0.78201202742
N1	H8	0.0027294124677
C2	H8	0.0090557845188
C3	H8	0.0002279506181
O4	H8	0.0021471212845
C5	H8	0.96225622955
C6	H8	0.042677123965
O7	H8	0.014340373253
N1	H9	0.00076999486581
C2	H9	0.0073104582327

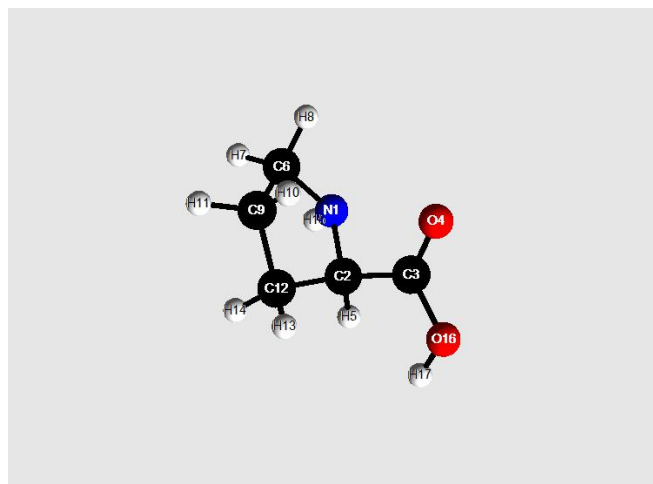
C3	H9	0.00041923159816
O4	H9	0.0013887629526
C5	H9	0.9584573423
C6	H9	0.040478282134
O7	H9	0.013383140024
H8	H9	0.043641759504
N1	N1	0.00037939440761
C2	N1	0.0023147236856
C3	N1	0.0012719094496
O4	N1	0.03807752408
C5	N1	0.94279168391
C6	N1	0.035680088835
O7	N1	0.014575101306
H8	N1	0.038515743328
H9	N1	0.038075447222
N1	H11	0.0060623249242
C2	H11	0.038352104907
C3	H11	0.0046499857114
O4	H11	0.012864208229
C5	H11	0.038465394684
C6	H11	0.90401803949
O7	H11	0.079120262773
H8	H11	0.0038161375098
H9	H11	0.010489954991
N1	H11	0.0024475886247
N1	H12	0.059242590843
C2	H12	0.90475399697
C3	H12	0.042781469989
O4	H12	0.014422591202
C5	H12	0.010352248797
C6	H12	0.033074989602
O7	H12	0.0077151757978
H8	H12	0.0011062763974
H9	H12	0.0080580019994
N1	H12	0.00049677450294
H11	H12	0.008933660043
N1	H13	0.0015773477195
C2	H13	0.006090413126
C3	H13	0.00085474140694
O4	H13	0.00012207437454
C5	H13	0.0040113739388
C6	H13	0.010210639367
O7	H13	0.60096349672
H8	H13	0.0033796212452
H9	H13	0.00020477354333
N1	H13	0.00036424034642
H11	H13	0.00067609097158
H12	H13	0.00016884932947



N1	H14	0.86695607667
C2	H14	0.021418321388
C3	H14	0.0016440921321
O4	H14	0.00062913158829
C5	H14	0.00044636913936
C6	H14	0.0044284016609
O7	H14	0.0033879469666
H8	H14	4.8037738481e-05
H9	H14	0.0002279643333
N1	H14	1.7574154348e-05
H11	H14	0.002463405381
H12	H14	0.0089449084376
H13	H14	3.5847821361e-05
N1	H15	0.8331756665
C2	H15	0.01890008957
C3	H15	0.0065106977012
O4	H15	0.0020470432505
C5	H15	0.00028576661231
C6	H15	0.0014414675167
O7	H15	0.013561577711
H8	H15	4.6301421414e-05
H9	H15	3.379718142e-05
N1	H15	3.7447272127e-05
H11	H15	0.00022125753394
H12	H15	0.0029051608086
H13	H15	0.000354953336
H14	H15	0.01596920699
N1	O16	0.082306596963
C2	O16	0.084887040213
C3	O16	0.73701863279
O4	O16	0.27862687057
C5	O16	0.00054850926546
C6	O16	0.0079807908718
O7	O16	0.0026252394495
H8	O16	0.0001333629862
H9	O16	0.00011920802162
N1	O16	0.00079764834702
H11	O16	0.00067765381396
H12	O16	0.0092616912885
H13	O16	0.00040006993735
H14	O16	0.0019395450308
H15	O16	0.0029501923651
N1	H17	0.044880216657
C2	H17	0.0023355747807
C3	H17	0.0062054444614
O4	H17	0.0077515833919
C5	H17	7.6543090042e-05
C6	H17	0.00061516390292

O7	H17	0.00024589355862
H8	H17	1.9750025642e-05
H9	H17	5.5147299355e-06
N1	H17	4.6040493441e-05
H11	H17	3.1192021224e-05
H12	H17	0.00013826902366
H13	H17	7.3372930023e-06
H14	H17	0.00069552465645
H15	H17	0.00089692896093
O16	H17	0.47951459503

## PROLINE



## HARTREE-FOCK

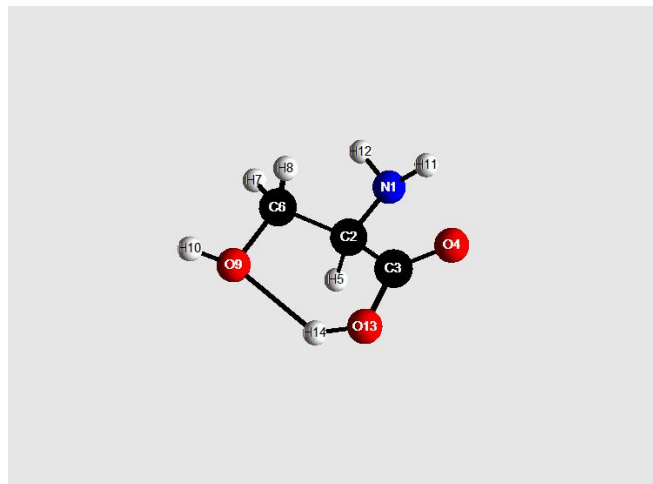
Atom A	Atom B	Delocalization index
N1	C2	0.96732662206
N1	C3	0.057574921679
C2	C3	0.85929833637
N1	O4	0.046282962302
C2	O4	0.090859415584
C3	O4	1.1318284398
N1	H5	0.058262379556
C2	H5	0.920972491
C3	H5	0.038349051241
O4	H5	0.012340792328
N1	C6	0.92590152168
C2	C6	0.029491819559
C3	C6	0.0017904054225
O4	C6	0.0058157487123
H5	C6	0.0067513778317
N1	H7	0.066112658631
C2	H7	0.0043374452885
C3	H7	0.00082008148155
O4	H7	0.00077148536535
H5	H7	0.00055616575058
C6	H7	0.93983459789
N1	H8	0.061258731872
C2	H8	0.0040334658355
C3	H8	0.00030796114752
O4	H8	0.0038697899915
H5	H8	0.0012111463339
C6	H8	0.93455517324
H7	H8	0.040666726902
N1	C9	0.06601795356
C2	C9	0.044690723871

C3	C9	0.0040177133143
O4	C9	0.01200069176
H5	C9	0.0078539580473
C6	C9	0.93814904832
H7	C9	0.040395404046
H8	C9	0.039055007695
N1	N1	0.0034991384177
C2	N1	0.0025537779986
C3	N1	0.0016903802581
O4	N1	0.016836067315
H5	N1	0.00041887263165
C6	N1	0.038570918438
H7	N1	0.0072912997259
H8	N1	0.0074812209577
C9	N1	0.9481455039
N1	H11	0.0086338430775
C2	H11	0.0088024029487
C3	H11	0.00088853723511
O4	H11	0.0014453496053
H5	H11	0.0014038674307
C6	H11	0.039474790038
H7	H11	0.0074777124597
H8	H11	0.0022539540291
C9	H11	0.96083066548
N1	H11	0.03994289037
N1	C12	0.074036924521
C2	C12	0.92138213652
C3	C12	0.045745720392
O4	C12	0.015525026566
H5	C12	0.036537287749
C6	C12	0.044881781231
H7	C12	0.0033009820559
H8	C12	0.0065942497727
C9	C12	0.9615365548
N1	C12	0.041274295195
H11	C12	0.041829230189
N1	H13	0.01264354716
C2	H13	0.037960614655
C3	H13	0.0063211091974
O4	H13	0.0023624855626
H5	H13	0.001345345966
C6	H13	0.00839254197
H7	H13	0.00066858520613
H8	H13	0.00099889427437
C9	H13	0.038171041985
N1	H13	0.00548253226
H11	H13	0.0014797966706
C12	H13	0.95581292945

N1	H14	0.0079460841716
C2	H14	0.042257747572
C3	H14	0.0082552712213
O4	H14	0.0031003165414
H5	H14	0.0067652987984
C6	H14	0.0032625419816
H7	H14	0.00088429962333
H8	H14	0.00054529496361
C9	H14	0.040366759563
N1	H14	0.0096509396571
H11	H14	0.0061577368302
C12	H14	0.95289717807
H13	H14	0.040928388975
N1	H15	0.8657123908
C2	H15	0.022360075817
C3	H15	0.0051287014417
O4	H15	0.001676605906
H5	H15	0.0049729453398
C6	H15	0.020855500439
H7	H15	0.005765203356
H8	H15	0.0033790189919
C9	H15	0.0034545080284
N1	H15	0.00036248169739
H11	H15	0.0005879899424
C12	H15	0.00224285958
H13	H15	0.00039694335425
H14	H15	0.00051189031256
N1	O16	0.011730504795
C2	O16	0.089793425304
C3	O16	0.71399346289
O4	O16	0.27276294711
H5	O16	0.021895607411
C6	O16	0.0010205625166
H7	O16	0.00034463004972
H8	O16	0.0002352691269
C9	O16	0.0015101284968
N1	O16	0.00046765333285
H11	O16	0.00035278258665
C12	O16	0.013126021847
H13	O16	0.0094510736684
H14	O16	0.0013746373817
H15	O16	0.0011234245263
N1	H17	0.00081379941391
C2	H17	0.0050679782183
C3	H17	0.0073982127427
O4	H17	0.010491824
H5	H17	0.0054504425861
C6	H17	0.00013028268674

H7	H17	1.3170765172e-05
H8	H17	5.4983098478e-05
C9	H17	0.00011048178987
N1	H17	1.885499643e-05
H11	H17	1.0802267018e-05
C12	H17	0.00045040624713
H13	H17	0.00031362603541
H14	H17	7.1640059056e-05
H15	H17	5.9851694331e-05
O16	H17	0.57129812634

## SERINE



### HARTREE-FOCK

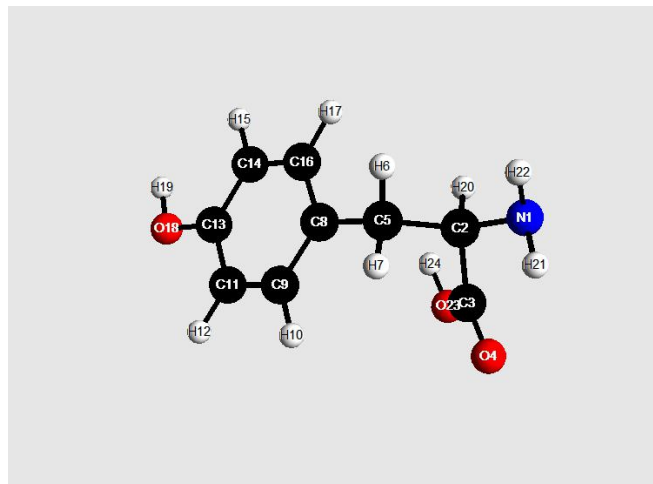
Atom A	Atom B	Delocalization index
N1	C2	0.98159820761
N1	C3	0.050767957044
C2	C3	0.85721455438
N1	O4	0.059633654627
C2	O4	0.09690308221
C3	O4	1.1124387276
N1	H5	0.061512803799
C2	H5	0.90515591983
C3	H5	0.039632944719
O4	H5	0.012457719036
N1	C6	0.074703174937
C2	C6	0.90503603985
C3	C6	0.041155994226
O4	C6	0.013425442525
H5	C6	0.037166624164
N1	H7	0.015243691906
C2	H7	0.036802105723
C3	H7	0.0079199113433
O4	H7	0.0028940711008
H5	H7	0.0030013708543
C6	H7	0.91507538762
N1	H8	0.010150474036
C2	H8	0.036683459525
C3	H8	0.0061518747195
O4	H8	0.0037910851344
H5	H8	0.0093772653836
C6	H8	0.91867169934
H7	H8	0.038495905552
N1	O9	0.014883141663
C2	O9	0.074269597107

C3	O9	0.0053805196045
O4	O9	0.0024993575158
H5	O9	0.017093160142
C6	O9	0.79747825879
H7	O9	0.078353902704
H8	O9	0.077808801349
N1	N1	0.0013994033324
C2	N1	0.0054675638468
C3	N1	0.00014649600832
O4	N1	0.00010679673528
H5	N1	0.00051324586409
C6	N1	0.010069088978
H7	N1	0.00062279856154
H8	N1	0.0012060051861
O9	N1	0.58726159693
N1	H11	0.80592747007
C2	H11	0.019255241398
C3	H11	0.0042342698282
O4	H11	0.031705239216
H5	H11	0.0061888877399
C6	H11	0.0018225511386
H7	H11	0.00044315720272
H8	H11	0.00034963620422
O9	H11	0.00069757514208
N1	H11	7.8152728059e-05
N1	H12	0.87266099356
C2	H12	0.021478610984
C3	H12	0.0058880353365
O4	H12	0.0027092078536
H5	H12	0.0012962648175
C6	H12	0.0087506185886
H7	H12	0.0072690752182
H8	H12	0.00067490977523
O9	H12	0.0012441760263
N1	H12	4.5473435339e-05
H11	H12	0.015144883556
N1	O13	0.011958293145
C2	O13	0.088647649759
C3	O13	0.73123270621
O4	O13	0.27721886533
H5	O13	0.0151099778
C6	O13	0.0099479331925
H7	O13	0.0012612683253
H8	O13	0.0018470850833
O9	O13	0.057453635233
N1	O13	0.00089999142781
H11	O13	0.0010798176777
H12	O13	0.0017475418325



N1	H14	0.00028372734336
C2	H14	0.0020210582886
C3	H14	0.0061188357591
O4	H14	0.0081487840272
H5	H14	0.00085783876641
C6	H14	0.00086998393995
H7	H14	0.00034837070366
H8	H14	9.5564741812e-05
O9	H14	0.035726059465
N1	H14	0.00065395532226
H11	H14	5.3101371214e-05
H12	H14	3.2640449648e-05
O13	H14	0.48677552515

## TYROSINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.97604663953
N1	C3	0.057575596951
C2	C3	0.85404751903
N1	O4	0.05405312072
C2	O4	0.094786149704
C3	O4	1.107847341
N1	C5	0.075605370251
C2	C5	0.92109697576
C3	C5	0.043033137291
O4	C5	0.018683161309
N1	H6	0.015479594941
C2	H6	0.040086647375
C3	H6	0.0084539185962
O4	H6	0.0032295788078
C5	H6	0.93971218569
N1	H7	0.01122866314
C2	H7	0.037682008392
C3	H7	0.0049199514866
O4	H7	0.010107322073
C5	H7	0.93877711558
H6	H7	0.03913836121
N1	C8	0.013197298434
C2	C8	0.042556589746
C3	C8	0.0052603850695
O4	C8	0.0015929331631
C5	C8	0.9910079647
H6	C8	0.042301003535
H7	C8	0.039587795643
N1	C9	0.0018501615013
C2	C9	0.0083952372462

C3	C9	0.0022666100753
O4	C9	0.002196107679
C5	C9	0.048288552199
H6	C9	0.0083704577388
H7	C9	0.011520500181
C8	C9	1.3467379567
N1	N1	0.00015567489211
C2	N1	0.00057841249805
C3	N1	0.0008717013073
O4	N1	0.0033487852355
C5	N1	0.0093280759576
H6	N1	0.00075690070358
H7	N1	0.0076571305851
C8	N1	0.044694683093
C9	N1	0.96376783681
N1	C11	0.00037088604325
C2	C11	0.001174548738
C3	C11	0.00021057597182
O4	C11	0.00027991457731
C5	C11	0.0076171674863
H6	C11	0.0014786891948
H7	C11	0.0008722808538
C8	C11	0.06901064629
C9	C11	1.4017996062
N1	C11	0.048241204586
N1	H12	5.672815123e-05
C2	H12	8.4439061291e-05
C3	H12	7.5840296965e-06
O4	H12	1.6060991251e-05
C5	H12	0.0010446805327
H6	H12	0.00020472934491
H7	H12	5.9882005846e-05
C8	H12	0.0081069342069
C9	H12	0.046157195688
N1	H12	0.0058249886208
C11	H12	0.96670055875
N1	C13	0.0006427834532
C2	C13	0.0031583167065
C3	C13	0.0002457314754
O4	C13	0.00012688890251
C5	C13	0.0042816672411
H6	C13	0.0017361003885
H7	C13	0.00077173663228
C8	C13	0.081445746751
C9	C13	0.076207911182
N1	C13	0.0081402049026
C11	C13	1.3004748105
H12	C13	0.045849397649

N1	C14	0.00032418810791
C2	C14	0.0011812395357
C3	C14	0.00028748068473
O4	C14	0.00018723970528
C5	C14	0.008093189123
H6	C14	0.0010029579515
H7	C14	0.0014612753833
C8	C14	0.070590638141
C9	C14	0.093754027117
N1	C14	0.0054270111148
C11	C14	0.06580185439
H12	C14	0.0067448910516
C13	C14	1.3232580292
N1	H15	4.7117816583e-05
C2	H15	6.988575361e-05
C3	H15	1.6679259492e-05
O4	H15	1.3259292445e-05
C5	H15	0.0011178407118
H6	H15	5.8501816278e-05
H7	H15	0.00024769483791
C8	H15	0.008499838247
C9	H15	0.0062384011505
N1	H15	0.00034948381475
C11	H15	0.0071823901994
H12	H15	0.0016890111104
C13	H15	0.04947656217
C14	H15	0.97434928391
N1	C16	0.0020978842062
C2	C16	0.011317714352
C3	C16	0.00077320199663
O4	C16	0.0004986475344
C5	C16	0.049601179036
H6	C16	0.011812154919
H7	C16	0.0075694107836
C8	C16	1.3710807008
C9	C16	0.076541185824
N1	C16	0.0083247366739
C11	C16	0.096421035448
H12	C16	0.0056344112215
C13	C16	0.073032281808
C14	C16	1.3811992907
H15	C16	0.048313848274
N1	H17	0.00036332614654
C2	H17	0.0020556271898
C3	H17	0.00018768038235
O4	H17	0.00015933507028
C5	H17	0.0093267284323
H6	H17	0.0061371651687

H7	H17	0.00077951489733
C8	H17	0.046397510984
C9	H17	0.0086501606191
N1	H17	0.0016472651842
C11	H17	0.0060400656427
H12	H17	0.00033562291316
C13	H17	0.0081822579052
C14	H17	0.049676312971
H15	H17	0.0061100491892
C16	H17	0.96935417898
N1	O18	0.00017386162663
C2	O18	0.00081361685939
C3	O18	6.158372631e-05
O4	O18	3.3943992023e-05
C5	O18	0.0011423921832
H6	O18	0.00046783787554
H7	O18	0.0002061063901
C8	O18	0.018269342951
C9	O18	0.013332524832
N1	O18	0.0013397688014
C11	O18	0.10855115733
H12	O18	0.015178604695
C13	O18	0.8313781423
C14	O18	0.11546805189
H15	O18	0.015634166662
C16	O18	0.014592315259
H17	O18	0.0016926444799
N1	H19	3.3187082919e-06
C2	H19	7.8027539575e-06
C3	H19	7.9773178436e-07
O4	H19	1.8625554833e-06
C5	H19	4.3603726545e-05
H6	H19	5.0464371845e-06
H7	H19	8.9443614946e-06
C8	H19	0.00024275170233
C9	H19	0.00093838470152
N1	H19	0.00019034761997
C11	H19	0.0055668465613
H12	H19	0.00034786093365
C13	H19	0.01014781574
C14	H19	0.0048250502504
H15	H19	0.003753145869
C16	H19	0.00039602451629
H17	H19	4.3523429047e-05
O18	H19	0.5772209449
N1	C2	0.062068487737
C2	C2	0.91009023749
C3	C2	0.035575336901

O4	C2	0.011255499195
C5	C2	0.038623209317
H6	C2	0.0032444462648
H7	C2	0.0096412762681
C8	C2	0.0087003940187
C9	C2	0.00068351009
N1	C2	0.00012088390122
C11	C2	0.00076943373979
H12	C2	4.1100595405e-05
C13	C2	0.00048193722263
C14	C2	0.00080143176946
H15	C2	2.8210863671e-05
C16	C2	0.0081724160072
H17	C2	0.0035224523155
O18	C2	0.00012065796931
H19	C2	1.3550777638e-06
N1	H21	0.82497776122
C2	H21	0.019810164633
C3	H21	0.0032459916234
O4	H21	0.024336699705
C5	H21	0.0021770281028
H6	H21	0.00031915532893
H7	H21	0.0012215310148
C8	H21	0.00033552149446
C9	H21	5.6433945932e-05
N1	H21	7.23631489e-06
C11	H21	2.1390506602e-05
H12	H21	2.054972331e-06
C13	H21	2.19431781e-05
C14	H21	1.9886798421e-05
H15	H21	1.8173706439e-06
C16	H21	0.00014989807905
H17	H21	5.3296825535e-05
O18	H21	6.601974648e-06
H19	H21	1.1851961629e-07
C2	H21	0.0082167603202
N1	H22	0.87495547178
C2	H22	0.021432600818
C3	H22	0.0072643186407
O4	H22	0.0030553085338
C5	H22	0.0071814761084
H6	H22	0.0060629017339
H7	H22	0.0004445179701
C8	H22	0.00057049618672
C9	H22	0.00019620051166
N1	H22	9.3368403954e-06
C11	H22	3.7111071446e-05
H12	H22	5.1232764071e-06

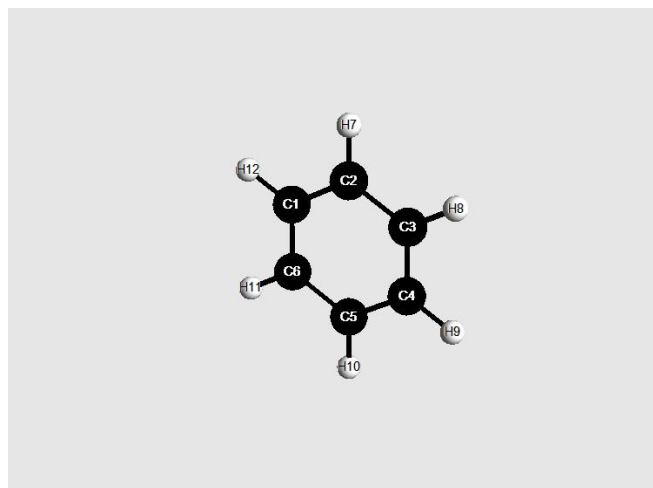
C13	H22	7.3358297594e-05
C14	H22	2.0585560098e-05
H15	H22	1.4543990029e-06
C16	H22	0.00015156221644
H17	H22	2.2824557196e-05
O18	H22	2.4078324609e-05
H19	H22	2.7085927127e-07
C2	H22	0.0010741940723
H21	H22	0.015780265654
N1	O23	0.010600851516
C2	O23	0.08762758691
C3	O23	0.72289796264
O4	O23	0.27719296678
C5	O23	0.0083318398351
H6	O23	0.0013363962708
H7	O23	0.00083215327417
C8	O23	0.019879361914
C9	O23	0.016937542455
N1	O23	0.0017450604283
C11	O23	0.002899756959
H12	O23	8.9838480618e-05
C13	O23	0.0010295065668
C14	O23	0.0013504590479
H15	O23	7.4156528854e-05
C16	O23	0.0039060616737
H17	O23	0.00012414251556
O18	O23	0.0002365591795
H19	O23	3.2244603445e-06
C2	O23	0.0211111453482
H21	O23	0.00091937271825
H22	O23	0.0017556616595
N1	H24	0.00063428398232
C2	H24	0.0041361007787
C3	H24	0.0069763792307
O4	H24	0.0098995621012
C5	H24	0.00036390421628
H6	H24	3.4628636041e-05
H7	H24	0.00013202257058
C8	H24	0.003740348239
C9	H24	0.00078154554385
N1	H24	2.2619376137e-05
C11	H24	0.00027936860935
H12	H24	1.3482616987e-05
C13	H24	0.00023566783538
C14	H24	0.00045952288062
H15	H24	1.2105298127e-05
C16	H24	0.0028109238481
H17	H24	0.00010989069564

O18	H24	5.3723025678e-05
H19	H24	4.8802635959e-07
C2	H24	0.0045221293914
H21	H24	0.00013000590273
H22	H24	3.5721932632e-05
O23	H24	0.5484319747



# AROMATICS

## BENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3873464851
C1	C3	0.074450464492
C2	C3	1.3873114675
C1	C4	0.099040563284
C2	C4	0.074447107776
C3	C4	1.3872776589
C1	C5	0.074447007146
C2	C5	0.099058091157
C3	C5	0.07446365239
C4	C5	1.3873454024
C1	C6	1.3872773485
C2	C6	0.074463896514
C3	C6	0.099066249145
C4	C6	0.07445042677
C5	C6	1.3873100803
C1	H7	0.049328668819
C2	H7	0.9771674034
C3	H7	0.049333529769
C4	H7	0.0086524673604
C5	H7	0.0063022175043
C6	H7	0.0086542528228
C1	H8	0.0086529335696
C2	H8	0.049322769992
C3	H8	0.97705319807
C4	H8	0.049343985334
C5	H8	0.0086527399843
C6	H8	0.0063029610675
H7	H8	0.0056650295194

C1	H9	0.0063018920447
C2	H9	0.0086532689307
C3	H9	0.049317981127
C4	H9	0.97713037641
C5	H9	0.049356087369
C6	H9	0.0086534376008
H7	H9	0.001383904079
H8	H9	0.0056648995818
C1	C1	0.0086524600502
C2	C1	0.0063022505187
C3	C1	0.0086542382062
C4	C1	0.049328683037
C5	C1	0.97716582566
C6	C1	0.049333584917
H7	C1	0.00041977391189
H8	C1	0.0013839056142
H9	C1	0.005665013681
C1	H11	0.049343849217
C2	H11	0.0086527494309
C3	H11	0.0063029659855
C4	H11	0.0086529328096
C5	H11	0.049322795231
C6	H11	0.97705363552
H7	H11	0.0013839059409
H8	H11	0.00041977057456
H9	H11	0.0013838738189
C1	H11	0.005665036837
C1	H12	0.97713035931
C2	H12	0.049355955561
C3	H12	0.008653443408
C4	H12	0.0063018905361
C5	H12	0.0086532763821
C6	H12	0.049318065354
H7	H12	0.0056650103245
H8	H12	0.0013838750221
H9	H12	0.00041977302326
C1	H12	0.0013839038948
H11	H12	0.0056648985845

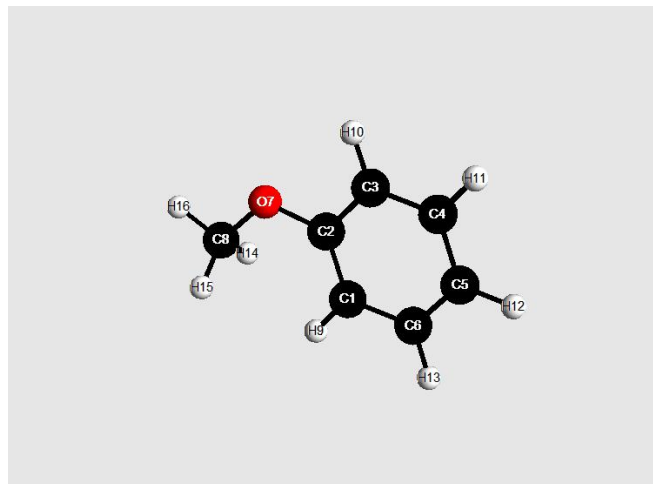
#### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.1602004377
C1	C3	0.052044056355
C2	C3	1.1601974879
C1	C4	0.060360766218
C2	C4	0.052066717021
C3	C4	1.1601825998
C1	C5	0.052066724326

C2	C5	0.060367970543
C3	C5	0.052046361291
C4	C5	1.1602005738
C1	C6	1.1601826254
C2	C6	0.052046372999
C3	C6	0.060318481085
C4	C6	0.052044074597
C5	C6	1.1601976763
C1	H7	0.036960099321
C2	H7	0.84073335263
C3	H7	0.036973689113
C4	H7	0.0066819171184
C5	H7	0.003805238206
C6	H7	0.0066809424412
C1	H8	0.0066813718585
C2	H8	0.036942945097
C3	H8	0.84088485686
C4	H8	0.036942198792
C5	H8	0.0066817074726
C6	H8	0.003804261357
H7	H8	0.0047015334887
C1	H9	0.0038050150384
C2	H9	0.0066820180453
C3	H9	0.036972992339
C4	H9	0.84071858131
C5	H9	0.036960782363
C6	H9	0.006681004661
H7	H9	0.0012912379696
H8	H9	0.0047014818458
C1	C1	0.0066819128831
C2	C1	0.0038052365762
C3	C1	0.0066809386203
C4	C1	0.036960107144
C5	C1	0.84073394431
C6	C1	0.036973697381
H7	C1	0.00032983958153
H8	C1	0.0012912397326
H9	C1	0.0047015351376
C1	H11	0.036942186739
C2	H11	0.0066817036494
C3	H11	0.0038042614296
C4	H11	0.0066813726403
C5	H11	0.036943003923
C6	H11	0.84088538956
H7	H11	0.0012912397702
H8	H11	0.00032983998315
H9	H11	0.001291235919
C1	H11	0.0047015317108

C1	H12	0.84071738893
C2	H12	0.036960704711
C3	H12	0.0066810063453
C4	H12	0.0038050106147
C5	H12	0.006682021773
C6	H12	0.036972994092
H7	H12	0.004701532391
H8	H12	0.001291236519
H9	H12	0.00032983863757
C1	H12	0.0012912370379
H11	H12	0.0047014823327

## ANISOLE



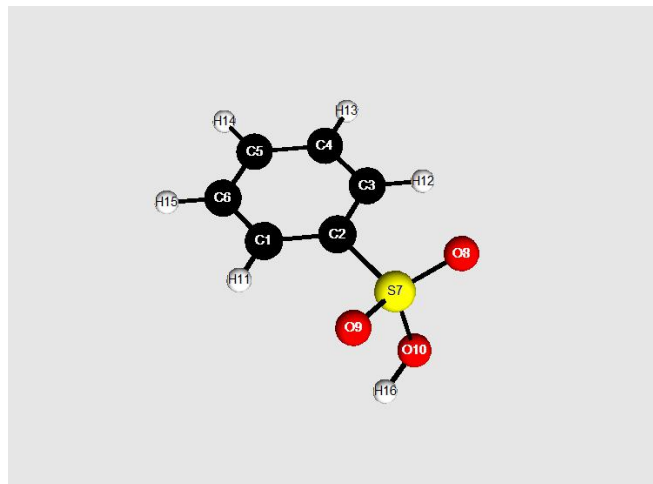
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3344407067
C1	C3	0.064986232853
C2	C3	1.2766672735
C1	C4	0.092704391648
C2	C4	0.074982903821
C3	C4	1.424880465
C1	C5	0.072716561397
C2	C5	0.08479454942
C3	C5	0.071972170998
C4	C5	1.354456193
C1	C6	1.3598489292
C2	C6	0.073923544139
C3	C6	0.097997105986
C4	C6	0.077938631745
C5	C6	1.4161423166
C1	O7	0.10618022409
C2	O7	0.82405308409
C3	O7	0.10912456723
C4	O7	0.013155421012
C5	O7	0.01868509282
C6	O7	0.013238037412
C1	C8	0.016881071237
C2	C8	0.020061239542
C3	C8	0.0068301853186
C4	C8	0.0015719385682
C5	C8	0.00080780997126
C6	C8	0.0014780165436
O7	C8	0.78787869713
C1	H9	0.96570478867
C2	H9	0.048257524193

C3	H9	0.0070505620382
C4	H9	0.0057956090311
C5	H9	0.0081469233452
C6	H9	0.046190813048
O7	H9	0.0089757480605
C8	H9	0.017727128785
C1	C1	0.0066536563208
C2	C1	0.0454205585
C3	C1	0.96818504512
C4	C1	0.047637198323
C5	C1	0.008453101173
C6	C1	0.0059495609508
O7	C1	0.017502606637
C8	C1	0.00055268588225
H9	C1	0.001644853845
C1	H11	0.005883710492
C2	H11	0.0085611086935
C3	H11	0.050870584903
C4	H11	0.97507604521
C5	H11	0.047076205566
C6	H11	0.0086357509506
O7	H11	0.0013640365953
C8	H11	0.00024134140412
H9	H11	0.00035804912079
C1	H11	0.0059395364031
C1	H12	0.0090968342521
C2	H12	0.0056612404353
C3	H12	0.0086714574328
C4	H12	0.048611213783
C5	H12	0.98014162759
C6	H12	0.051337755038
O7	H12	0.0014737261465
C8	H12	0.00010670743672
H9	H12	0.0012199410804
C1	H12	0.0012955117318
H11	H12	0.0054251422354
C1	H13	0.048827104376
C2	H13	0.0083007711783
C3	H13	0.0063154374894
C4	H13	0.0089733356647
C5	H13	0.049658160969
C6	H13	0.97524615658
O7	H13	0.0017984598097
C8	H13	5.9537471347e-05
H9	H13	0.0059385351386
C1	H13	0.00036854310828
H11	H13	0.0015012385819
H12	H13	0.0057611690254

C1	H14	0.011327760143
C2	H14	0.0045368788578
C3	H14	0.0010960077182
C4	H14	0.00061465936351
C5	H14	0.00095623358447
C6	H14	0.0010415679111
O7	H14	0.076759794238
C8	H14	0.92319641147
H9	H14	0.010604374697
C1	H14	0.00013354049382
H11	H14	3.6762883952e-05
H12	H14	9.0059203632e-05
H13	H14	4.5171513165e-05
C1	H15	0.011367223696
C2	H15	0.0045202053658
C3	H15	0.0010963305001
C4	H15	0.00061737359056
C5	H15	0.00095934401214
C6	H15	0.0010440881868
O7	H15	0.076738865879
C8	H15	0.92311841232
H9	H15	0.010591522735
C1	H15	0.00013315056619
H11	H15	3.688178504e-05
H12	H15	9.0169773953e-05
H13	H15	4.520950653e-05
H14	H15	0.039984754572
C1	H16	0.001988251747
C2	H16	0.0067559253307
C3	H16	0.00087061746419
C4	H16	0.00025034324051
C5	H16	0.00012810164586
C6	H16	0.00016685020239
O7	H16	0.071643807156
C8	H16	0.93029181688
H9	H16	0.0021785266934
C1	H16	7.8406968918e-05
H11	H16	5.7174671199e-05
H12	H16	1.706968554e-05
H13	H16	2.9322298661e-05
H14	H16	0.037307630944
H15	H16	0.037298206687

## BENZENESULFONIC ACID



### HARTREE-FOCK

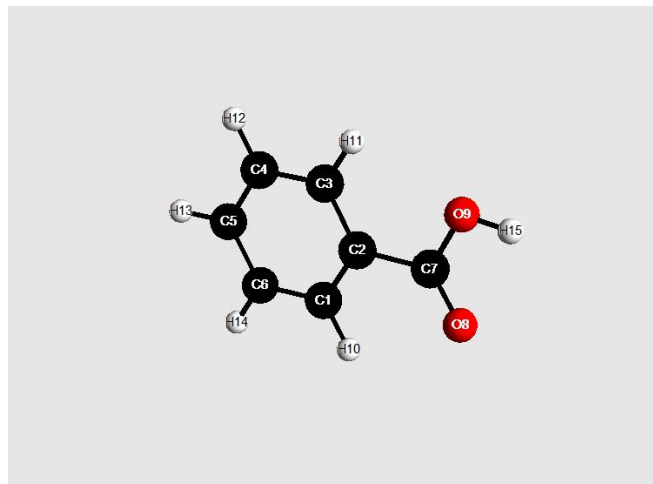
Atom A	Atom B	Delocalization index
C1	C2	1.3723926659
C1	C3	0.065073290854
C2	C3	1.3561132999
C1	C4	0.095617604035
C2	C4	0.076624363484
C3	C4	1.3950489827
C1	C5	0.077107977745
C2	C5	0.09570329796
C3	C5	0.077058938045
C4	C5	1.376504239
C1	C6	1.3810577836
C2	C6	0.076254145258
C3	C6	0.096428500727
C4	C6	0.072463711203
C5	C6	1.3903320821
C1	S7	0.043925628322
C2	S7	0.85885438098
C3	S7	0.042878032096
C4	S7	0.0075051129278
C5	S7	0.0063816616439
C6	S7	0.0074417043237
C1	O8	0.012461153641
C2	O8	0.099767668245
C3	O8	0.028138740874
C4	O8	0.0025239650792
C5	O8	0.0028573697173
C6	O8	0.002984712967
S7	O8	0.95225652714
C1	O9	0.030606386128
C2	O9	0.096168115549



C3	O9	0.011574004934
C4	O9	0.0030283925867
C5	O9	0.0022788110662
C6	O9	0.002565505921
S7	O9	0.93326800659
O8	O9	0.19990664621
C1	C1	0.012475128313
C2	C1	0.0874132792
C3	C1	0.013884784991
C4	C1	0.0019951015904
C5	C1	0.0041848249532
C6	C1	0.0020436188784
S7	C1	0.63783422797
O8	C1	0.18856860039
O9	C1	0.21060559508
C1	H11	0.95053803618
C2	H11	0.044931236721
C3	H11	0.0076031577133
C4	H11	0.00516693365
C5	H11	0.0076033840455
C6	H11	0.042545608693
S7	H11	0.0051291373684
O8	H11	0.0011326854454
O9	H11	0.028070038157
C1	H11	0.00099109949125
C1	H12	0.0075619365529
C2	H12	0.044338936038
C3	H12	0.95152660335
C4	H12	0.043005598108
C5	H12	0.0076882956898
C6	H12	0.0050768840161
S7	H12	0.0050959841027
O8	H12	0.022542318894
O9	H12	0.0010064099278
C1	H12	0.0016409116441
H11	H12	0.0013639991102
C1	H13	0.0055987709736
C2	H13	0.0087286115672
C3	H13	0.049018953773
C4	H13	0.97275179751
C5	H13	0.047546241532
C6	H13	0.0082483100085
S7	H13	0.0011491700145
O8	H13	0.0001270911016
O9	H13	0.0005790211682
C1	H13	0.00017762337643
H11	H13	0.0003139210452
H12	H13	0.0053290864004

C1	H14	0.0084433737835
C2	H14	0.0055861878168
C3	H14	0.0083541354898
C4	H14	0.04716291302
C5	H14	0.97217655431
C6	H14	0.047723222998
S7	H14	0.00038564690716
O8	H14	0.00022684622261
O9	H14	0.00020685571785
C1	H14	0.00025147109581
H11	H14	0.0011661384929
H12	H14	0.0011720955922
H13	H14	0.0054017816169
C1	H15	0.048668968087
C2	H15	0.008709265396
C3	H15	0.0056940482315
C4	H15	0.0083273761137
C5	H15	0.048080883388
C6	H15	0.97313089484
S7	H15	0.0011595028329
O8	H15	0.00054324800943
O9	H15	0.00011691774503
C1	H15	0.0002200503876
H11	H15	0.0052715028006
H12	H15	0.00031205896928
H13	H15	0.0013017503244
H14	H15	0.0054658544725
C1	H16	0.00021831521932
C2	H16	0.0011643911886
C3	H16	0.00015645909266
C4	H16	3.776276617e-05
C5	H16	4.9470842549e-05
C6	H16	5.4420617575e-05
S7	H16	0.0067983408859
O8	H16	0.0082097720349
O9	H16	0.0064313315022
C1	H16	0.51956681444
H11	H16	3.3891608011e-05
H12	H16	1.9344525579e-05
H13	H16	2.9940740158e-06
H14	H16	3.07215165e-06
H15	H16	8.3958592011e-06

## BENZOIC ACID



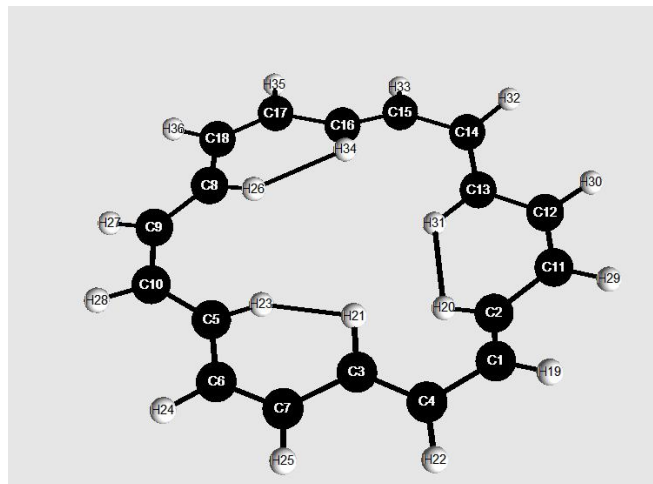
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3451914085
C1	C3	0.06803600938
C2	C3	1.3571330719
C1	C4	0.095724886519
C2	C4	0.072658988883
C3	C4	1.389134767
C1	C5	0.07683891905
C2	C5	0.093322923453
C3	C5	0.076677652641
C4	C5	1.3869890281
C1	C6	1.3987064774
C2	C6	0.073255630231
C3	C6	0.095029856859
C4	C6	0.072053411865
C5	C6	1.3781354773
C1	C7	0.051444869061
C2	C7	0.93947798256
C3	C7	0.049508969174
C4	C7	0.0074917879398
C5	C7	0.0092960988989
C6	C7	0.00760696731
C1	O8	0.040556525281
C2	O8	0.10682406111
C3	O8	0.021202492168
C4	O8	0.0037517556653
C5	O8	0.0082669936954
C6	O8	0.0033955778359
C7	O8	1.0946941722
C1	O9	0.010728379756
C2	O9	0.08603269702

C3	O9	0.03306831819
C4	O9	0.002744840277
C5	O9	0.0031645267529
C6	O9	0.0025096292051
C7	O9	0.71423173192
O8	O9	0.29166053471
C1	C1	0.95233286043
C2	C1	0.042050407032
C3	C1	0.0077407858933
C4	C1	0.0050997560861
C5	C1	0.0077718830738
C6	C1	0.043953018407
C7	C1	0.0051818789837
O8	C1	0.027451986163
O9	C1	0.0011348173395
C1	H11	0.0079295003888
C2	H11	0.04324633776
C3	H11	0.95624323745
C4	H11	0.044731034614
C5	H11	0.0078300145033
C6	H11	0.0053109672984
C7	H11	0.0043342560352
O8	H11	0.0013919314977
O9	H11	0.027567147391
C1	H11	0.0013925117707
C1	H12	0.0058825082483
C2	H12	0.0085676052087
C3	H12	0.049369449047
C4	H12	0.97571819562
C5	H12	0.04892296299
C6	H12	0.0084484119037
C7	H12	0.0010867323298
O8	H12	0.00054013803051
O9	H12	0.00010132436472
C1	H12	0.00032677831573
H11	H12	0.0054834760063
C1	H13	0.0084263070503
C2	H13	0.0056343087021
C3	H13	0.0084888017652
C4	H13	0.048130655534
C5	H13	0.97393160701
C6	H13	0.047660087963
C7	H13	0.00050563790164
O8	H13	0.0005888236708
O9	H13	0.00025024769491
C1	H13	0.0012138740705
H11	H13	0.0012099076513
H12	H13	0.0055451656178

C1	H14	0.049483962508
C2	H14	0.0086155859301
C3	H14	0.005782938935
C4	H14	0.0083969165803
C5	H14	0.048535678313
C6	H14	0.9752456873
C7	H14	0.0010727814684
O8	H14	0.00012669375436
O9	H14	0.00040423342373
C1	H14	0.0053594996563
H11	H14	0.00033779695612
H12	H14	0.0013449908414
H13	H14	0.0054897844728
C1	H15	0.00078578652344
C2	H15	0.0059811969481
C3	H15	0.00074110996306
C4	H15	3.8926569564e-05
C5	H15	5.9337943609e-05
C6	H15	0.0001761425327
C7	H15	0.0078039005029
O8	H15	0.010910716951
O9	H15	0.53992808837
C1	H15	4.1041222878e-05
H11	H15	0.00060667907185
H12	H15	7.1542673348e-06
H13	H15	4.89374432e-06
H14	H15	4.7895153274e-05

## (18)ANNULENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.707429091
C1	C3	0.067815612821
C2	C3	0.056051697554
C1	C4	1.0802573435
C2	C4	0.066815454323
C3	C4	1.7077220284
C1	C5	0.00046753498363
C2	C5	0.00057221832075
C3	C5	0.016059053226
C4	C5	0.0040814585241
C1	C6	0.0042763154949
C2	C6	0.0085334881329
C3	C6	0.066641062722
C4	C6	0.058424203234
C5	C6	1.0961583292
C1	C7	0.010416398298
C2	C7	0.0043110825024
C3	C7	1.0963249291
C4	C7	0.067635587288
C5	C7	0.066684328139
C6	C7	1.7003134827
C1	C8	0.00017289750138
C2	C8	0.0004345729973
C3	C8	0.0005722109772
C4	C8	0.0017014492385
C5	C8	0.056028983469
C6	C8	0.0043090015477
C7	C8	0.0085351885731
C1	C9	0.00021106034774
C2	C9	0.00017294256019

C3	C9	0.00046768153504
C4	C9	0.00065705587538
C5	C9	0.067868530364
C6	C9	0.01041543046
C7	C9	0.0042784535952
C8	C9	1.7073917701
C1	C1	0.00065674361819
C2	C1	0.001701182248
C3	C1	0.0040798865284
C4	C1	0.0084617711674
C5	C1	1.7076475241
C6	C1	0.067588331543
C7	C1	0.05843132255
C8	C1	0.066762940712
C9	C1	1.0803444308
C1	C11	0.068710248998
C2	C11	1.0973296938
C3	C11	0.0042480954773
C4	C11	0.010449853491
C5	C11	0.00022288431816
C6	C11	0.00072019273948
C7	C11	0.00059355685388
C8	C11	0.00016820267916
C9	C11	0.00048680355371
C1	C11	0.00018651841039
C1	C12	0.05961395789
C2	C12	0.066213612489
C3	C12	0.0085547235719
C4	C12	0.0043461781889
C5	C12	0.00017548350266
C6	C12	0.0021705768017
C7	C12	0.00072721004716
C8	C12	0.00023156554355
C9	C12	0.00018339212508
C1	C12	0.00053743972677
C11	C12	1.6987980908
C1	C13	0.0040762001013
C2	C13	0.01491577032
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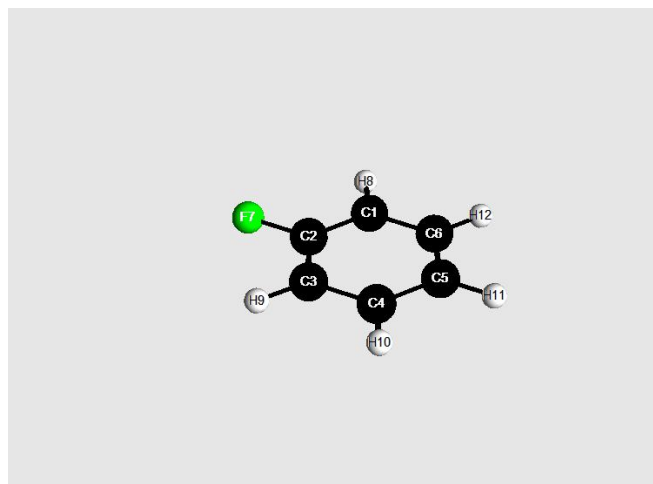


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C14	H35	0.0007491051296
C15	H35	0.0087202734811
C16	H35	0.040131002166
C17	H35	0.96818965123
C18	H35	0.060978969409
H19	H35	1.0372702006e-06
C2	H35	4.4596464986e-06
H21	H35	6.3408827697e-06
H22	H35	1.9881568531e-06
H23	H35	3.715005605e-05
H24	H35	4.6142662039e-06
H25	H35	9.2568837702e-06
H26	H35	0.00035283888678
H27	H35	0.00021826030953
H28	H35	9.1854222571e-05
H29	H35	3.8860307949e-06
C3	H35	6.3644698904e-06
H31	H35	0.00023467783075
H32	H35	3.5558975516e-05
H33	H35	0.0062303530641
H34	H35	0.0084626543333
C1	H36	3.2377978904e-05
C2	H36	1.1170160759e-05
C3	H36	1.4512245056e-05
C4	H36	1.1300814414e-05
C5	H36	0.00046198899269
C6	H36	7.4431612119e-05
C7	H36	4.7029005485e-05
C8	H36	0.040151020628
C9	H36	0.0088718021249
C1	H36	0.00073736283591
C11	H36	0.00014153659863

C12	H36	4.7076661023e-05
C13	H36	0.00054821694762
C14	H36	0.00044802734382
C15	H36	0.0040957873547
C16	H36	0.0098290648973
C17	H36	0.060935229724
C18	H36	0.96800780981
H19	H36	1.7223238104e-06
C2	H36	1.9588979894e-06
H21	H36	1.2095418384e-05
H22	H36	1.0098863395e-06
H23	H36	0.00027000864281
H24	H36	6.9292124115e-06
H25	H36	4.3299821455e-06
H26	H36	0.0083471648693
H27	H36	0.006278028613
H28	H36	3.3460653288e-05
H29	H36	9.1353353317e-06
C3	H36	3.8851864184e-06
H31	H36	3.9433656636e-05
H32	H36	9.8818606987e-05
H33	H36	0.00021829005259
H34	H36	0.00034418556576
H35	H36	0.0081620563895

## FLUROBENZENE

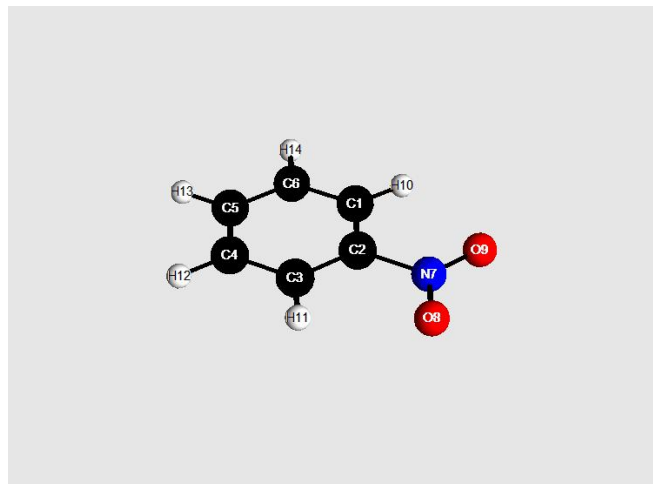


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3335393189
C1	C3	0.061965631846
C2	C3	1.3334755602
C1	C4	0.097983524981
C2	C4	0.079867079391
C3	C4	1.3828003788
C1	C5	0.072435144997
C2	C5	0.090255455221
C3	C5	0.072421434314
C4	C5	1.3879840249
C1	C6	1.3827833546
C2	C6	0.079894632385
C3	C6	0.097988659286
C4	C6	0.077287567792
C5	C6	1.3879608232
C1	F7	0.10148093958
C2	F7	0.72264435742
C3	F7	0.10146128241
C4	F7	0.012688951954
C5	F7	0.014640423914
C6	F7	0.012690665907
C1	H8	0.96766385264
C2	H8	0.048675550939
C3	H8	0.0064686695916
C4	H8	0.0059171151118
C5	H8	0.0081866031546
C6	H8	0.044682772182
F7	H8	0.01259611358
C1	H9	0.0064702418449
C2	H9	0.048651620863

C3	H9	0.96765618475
C4	H9	0.044705677189
C5	H9	0.0081859330746
C6	H9	0.0059196666735
F7	H9	0.012596244469
H8	H9	0.0015429849856
C1	C1	0.0060256580751
C2	C1	0.0086079983411
C3	C1	0.048921109857
C4	C1	0.97394821803
C5	C1	0.04781816757
C6	C1	0.0086307685033
F7	C1	0.0015781204984
H8	C1	0.00034658816012
H9	C1	0.0055464666769
C1	H11	0.0086737919506
C2	H11	0.0058084871468
C3	H11	0.0086725199185
C4	H11	0.049418674301
C5	H11	0.97713270314
C6	H11	0.049420880343
F7	H11	0.0011072270147
H8	H11	0.0012636743835
H9	H11	0.001263676802
C1	H11	0.0055470688027
C1	H12	0.048913510222
C2	H12	0.0086080619121
C3	H12	0.0060241497998
C4	H12	0.0086289064494
C5	H12	0.047795597698
C6	H12	0.97388076247
F7	H12	0.0015781194062
H8	H12	0.0055464609622
H9	H12	0.00034659070038
C1	H12	0.0014511181194
H11	H12	0.0055470641725

## NITROBENZENE



## HARTREE-FOCK

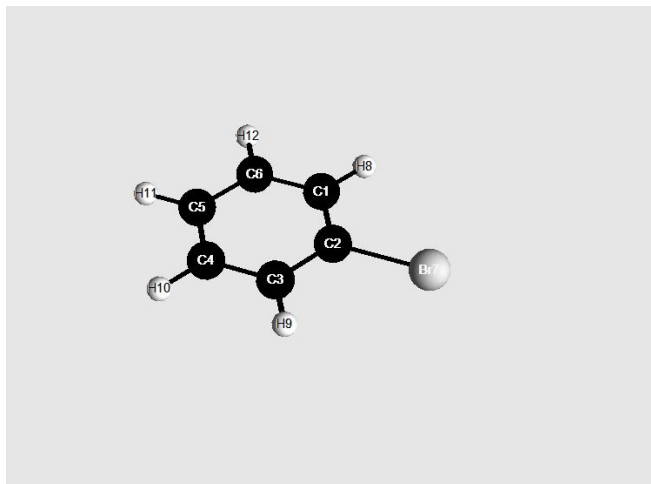
Atom A	Atom B	Delocalization index
C1	C2	1.3297005779
C1	C3	0.061860613659
C2	C3	1.3296890327
C1	C4	0.094873815906
C2	C4	0.077321844811
C3	C4	1.3894418853
C1	C5	0.077243326103
C2	C5	0.089716676739
C3	C5	0.077234052444
C4	C5	1.3823056439
C1	C6	1.3894286096
C2	C6	0.077331192258
C3	C6	0.094870411845
C4	C6	0.072363087752
C5	C6	1.3822519278
C1	N7	0.067429335939
C2	N7	0.79891742341
C3	N7	0.067452650108
C4	N7	0.0091220655325
C5	N7	0.011372316893
C6	N7	0.009121317005
C1	O8	0.01864812729
C2	O8	0.073729041195
C3	O8	0.043816123358
C4	O8	0.0035055406475
C5	O8	0.00668266057
C6	O8	0.0039132324297
N7	O8	1.6810634514
C1	O9	0.043872983077
C2	O9	0.073709514832

C3	O9	0.018645833588
C4	O9	0.0039130427086
C5	O9	0.0066829369709
C6	O9	0.0035055548099
N7	O9	1.6810134006
O8	O9	0.32348567941
C1	C1	0.94338751097
C2	C1	0.042172781234
C3	C1	0.006859797507
C4	C1	0.0048386857597
C5	C1	0.0074269401159
C6	C1	0.040683862597
N7	C1	0.0056962271176
O8	C1	0.0019275387093
O9	C1	0.032560535778
C1	H11	0.0068612325004
C2	H11	0.04217514535
C3	H11	0.94336574441
C4	H11	0.040699516179
C5	H11	0.0074264494183
C6	H11	0.0048396837941
N7	H11	0.00570120503
O8	H11	0.032562261804
O9	H11	0.0019273736801
C1	H11	0.0013902470709
C1	H12	0.0055680835047
C2	H12	0.0085331583056
C3	H12	0.048915071471
C4	H12	0.97253891952
C5	H12	0.047606400198
C6	H12	0.0082723275822
N7	H12	0.0012897333776
O8	H12	0.00014040589194
O9	H12	0.0005698156837
C1	H12	0.00028260235686
H11	H12	0.0052529769576
C1	H13	0.0083809495829
C2	H13	0.005330530546
C3	H13	0.0083798582845
C4	H13	0.047176505811
C5	H13	0.97169134395
C6	H13	0.047172631319
N7	H13	0.00063527221243
O8	H13	0.00045909866756
O9	H13	0.00045910108081
C1	H13	0.0011129280319
H11	H13	0.0011129372981
H12	H13	0.0053904028969

C1	H14	0.048910993587
C2	H14	0.0085331119132
C3	H14	0.0055668576493
C4	H14	0.008271785193
C5	H14	0.04758021263
C6	H14	0.97247695913
N7	H14	0.0012896468447
O8	H14	0.00056981658459
O9	H14	0.00014040743847
C1	H14	0.0052529835822
H11	H14	0.00028260289242
H12	H14	0.0013307014808
H13	H14	0.0053903996373



## BROMOBENZENE

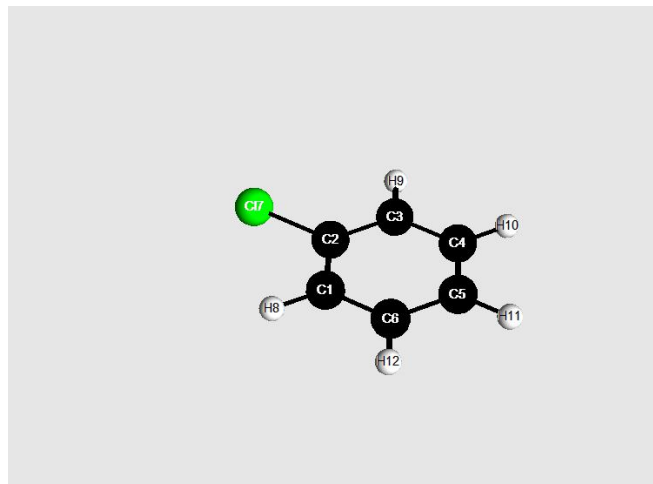


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3710777984
C1	C3	0.063645559806
C2	C3	1.3710067642
C1	C4	0.09707806359
C2	C4	0.078814304889
C3	C4	1.3819146144
C1	C5	0.073024918729
C2	C5	0.096128794011
C3	C5	0.073018292253
C4	C5	1.3866608437
C1	C6	1.3818944797
C2	C6	0.078833650458
C3	C6	0.097088171086
C4	C6	0.075470850512
C5	C6	1.3866287256
C1	Br7	0.089130203689
C2	Br7	1.1200026843
C3	Br7	0.089103593661
C4	Br7	0.016389294412
C5	Br7	0.014765062774
C6	Br7	0.016391604477
C1	H8	0.962656695
C2	H8	0.048657569604
C3	H8	0.0073324323815
C4	H8	0.0056734936814
C5	H8	0.0079337048969
C6	H8	0.045088874648
Br7	H8	0.023537862865
C1	H9	0.0073334063999
C2	H9	0.048619561548

C3	H9	0.96264085143
C4	H9	0.045112227614
C5	H9	0.0079330639219
C6	H9	0.005675364641
Br7	H9	0.02353845719
H8	H9	0.0014004036372
C1	C1	0.0059183393921
C2	C1	0.0087571011291
C3	C1	0.048931211356
C4	C1	0.97359870021
C5	C1	0.047941125467
C6	C1	0.0085296997539
Br7	C1	0.0023446681862
H8	C1	0.00034519079934
H9	C1	0.0056056167154
C1	H11	0.0084760145916
C2	H11	0.0059236463651
C3	H11	0.0084753447027
C4	H11	0.048628177579
C5	H11	0.9753712093
C6	H11	0.048631559763
Br7	H11	0.001258278726
H8	H11	0.0012266619906
H9	H11	0.0012266688796
C1	H11	0.0054981946533
C1	H12	0.048931599203
C2	H12	0.0087570090811
C3	H12	0.0059175027379
C4	H12	0.0085285201203
C5	H12	0.047914460939
C6	H12	0.97353878859
Br7	H12	0.0023446673553
H8	H12	0.0056055857153
H9	H12	0.00034519853307
C1	H12	0.0014086769447
H11	H12	0.0054981782805

## CHLOROBENZENE

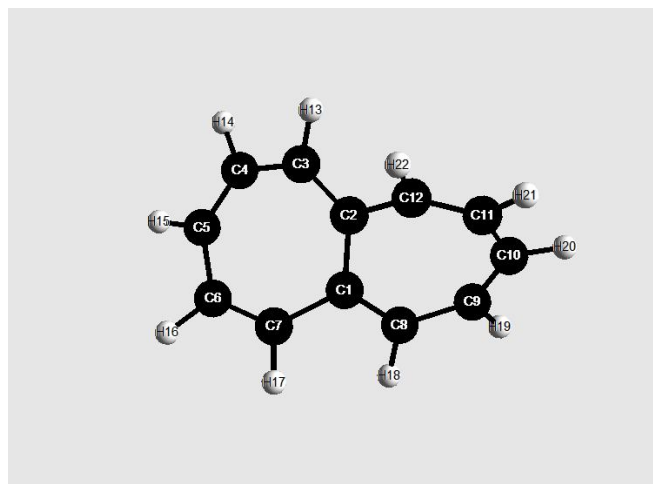


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.35952819
C1	C3	0.062753567341
C2	C3	1.3595029078
C1	C4	0.097072082502
C2	C4	0.078467817386
C3	C4	1.3829659226
C1	C5	0.072804729056
C2	C5	0.094551728034
C3	C5	0.072795991462
C4	C5	1.3867028054
C1	C6	1.3829489549
C2	C6	0.07848681388
C3	C6	0.097081110299
C4	C6	0.075724394545
C5	C6	1.3866727198
C1	Cl7	0.095674877078
C2	Cl7	1.0823389638
C3	Cl7	0.095694149973
C4	Cl7	0.015751316489
C5	Cl7	0.016090902887
C6	Cl7	0.015753645083
C1	H8	0.96337557668
C2	H8	0.047948630677
C3	H8	0.0071511318283
C4	H8	0.0056838573575
C5	H8	0.0079695926242
C6	H8	0.045019381485
Cl7	H8	0.021790003677
C1	H9	0.0071523600805
C2	H9	0.04793489599

C3	H9	0.96339846171
C4	H9	0.045041545881
C5	H9	0.0079688621921
C6	H9	0.0056858288563
Cl7	H9	0.02179125493
H8	H9	0.001451401666
C1	C1	0.0059371814835
C2	C1	0.0087093800098
C3	C1	0.04897229498
C4	C1	0.97378131262
C5	C1	0.047941593328
C6	C1	0.0085464822491
Cl7	C1	0.0021342088773
H8	C1	0.00034376220844
H9	C1	0.0055874143746
C1	H11	0.0085094599921
C2	H11	0.0058844369625
C3	H11	0.0085088058309
C4	H11	0.048769141539
C5	H11	0.97572896535
C6	H11	0.048772557391
Cl7	H11	0.0013116007852
H8	H11	0.0012349067825
H9	H11	0.0012349040193
C1	H11	0.0055104917729
C1	H12	0.048972123148
C2	H12	0.0087093199438
C3	H12	0.0059360477549
C4	H12	0.0085450054193
C5	H12	0.047915694542
C6	H12	0.97371943886
Cl7	H12	0.0021342056976
H8	H12	0.0055874182072
H9	H12	0.00034375961766
C1	H12	0.0014139912376
H11	H12	0.0055104701931

## HEPTALENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.0284821146
C1	C3	0.059443269696
C2	C3	1.6703657643
C1	C4	0.013636016672
C2	C4	0.06536425932
C3	C4	1.1012522753
C1	C5	0.0132135053
C2	C5	0.056097427401
C3	C5	0.064191898801
C4	C5	1.6999681606
C1	C6	0.060469557637
C2	C6	0.016635430078
C3	C6	0.015821518646
C4	C6	0.06633527312
C5	C6	1.0958794769
C1	C7	1.0368662092
C2	C7	0.062908181226
C3	C7	0.018688859385
C4	C7	0.060276351923
C5	C7	0.066906521759
C6	C7	1.7237089586
C1	C8	1.6704495099
C2	C8	0.059333933162
C3	C8	0.033513494182
C4	C8	0.0058137832854
C5	C8	0.0059399644378
C6	C8	0.035290983781
C7	C8	0.069618707589
C1	C9	0.065345473874
C2	C9	0.013619214764

C3	C9	0.005808915966
C4	C9	0.00088667703303
C5	C9	0.0010225862607
C6	C9	0.0034857511242
C7	C9	0.0092731803557
C8	C9	1.1012955659
C1	C1	0.056091307625
C2	C1	0.013209192511
C3	C1	0.0059383784221
C4	C1	0.0010229195339
C5	C1	0.0012714184866
C6	C1	0.0053532977892
C7	C1	0.0038038324111
C8	C1	0.064229953713
C9	C1	1.69993387
C1	C11	0.016648108544
C2	C11	0.060280349294
C3	C11	0.035268228442
C4	C11	0.0034850362869
C5	C11	0.005351442287
C6	C11	0.0014916831597
C7	C11	0.0022152598704
C8	C11	0.015824808587
C9	C11	0.066292926577
C1	C11	1.0957925609
C1	C12	0.06292147349
C2	C12	1.0366233136
C3	C12	0.069587230827
C4	C12	0.009276129761
C5	C12	0.0038034736353
C6	C12	0.0022158103723
C7	C12	0.006114852065
C8	C12	0.018697014457
C9	C12	0.060271835327
C1	C12	0.066908534271
C11	C12	1.7236642794
C1	H13	0.010334476005
C2	H13	0.062577961785
C3	H13	0.96309801017
C4	H13	0.041170301308
C5	H13	0.0090073744117
C6	H13	0.00089699079606
C7	H13	0.0012995511797
C8	H13	0.0029087610908
C9	H13	0.00063057244905
C1	H13	0.00058248930098
C11	H13	0.0035538343352
C12	H13	0.016793516692

C1	H14	0.00078813236551
C2	H14	0.0088172239081
C3	H14	0.041028878094
C4	H14	0.97098864309
C5	H14	0.063581498322
C6	H14	0.010196686503
C7	H14	0.0039108215667
C8	H14	0.00052618966444
C9	H14	6.9214321261e-05
C1	H14	0.00010067531334
C11	H14	0.00031163842718
C12	H14	0.0010704136957
H13	H14	0.005481125248
C1	H15	0.00072835243416
C2	H15	0.0036841337303
C3	H15	0.010146514096
C4	H15	0.063898863407
C5	H15	0.97303091954
C6	H15	0.04079010091
C7	H15	0.0087455390108
C8	H15	0.00052252674893
C9	H15	9.0325688247e-05
C1	H15	0.00011012326895
C11	H15	0.0004204931602
C12	H15	0.00039672099152
H13	H15	0.001275882865
H14	H15	0.008930696061
C1	H16	0.010279187073
C2	H16	0.0012390808939
C3	H16	0.00088782735224
C4	H16	0.0088991101292
C5	H16	0.040580034921
C6	H16	0.97008961929
C7	H16	0.065423156762
C8	H16	0.002914524062
C9	H16	0.00041004229152
C1	H16	0.00039238252995
C11	H16	0.00011822579174
C12	H16	0.0002123619992
H13	H16	9.9115871464e-05
H14	H16	0.0013359470719
H15	H16	0.0051476462292
C1	H17	0.039792490172
C2	H17	0.005455724804
C3	H17	0.0015549884045
C4	H17	0.0037234055886
C5	H17	0.010280843755
C6	H17	0.062955015894

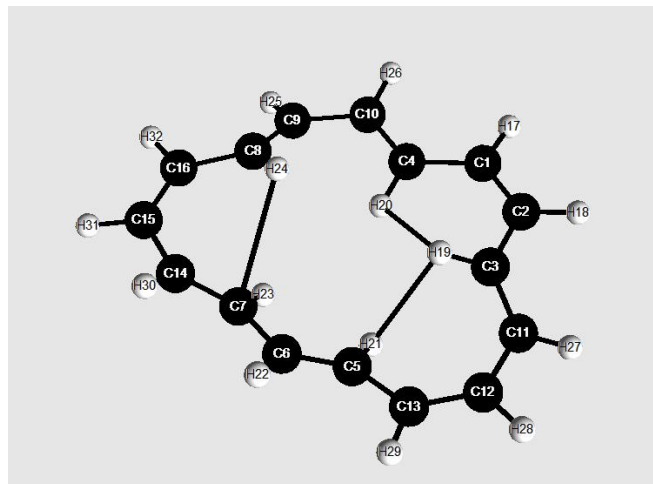
C7	H17	0.96497543221
C8	H17	0.01362010983
C9	H17	0.00088152897496
C1	H17	0.0013777453556
C11	H17	0.0002057458217
C12	H17	0.00087015603425
H13	H17	0.00015368285096
H14	H17	0.00035603232876
H15	H17	0.0013229033449
H16	H17	0.0089381072145
C1	H18	0.0625843729
C2	H18	0.010329315194
C3	H18	0.0029081644028
C4	H18	0.00063067656047
C5	H18	0.00058245385448
C6	H18	0.0035543752215
C7	H18	0.016764716677
C8	H18	0.96316752156
C9	H18	0.041170703565
C1	H18	0.0090070381118
C11	H18	0.00089693144198
C12	H18	0.0012998779768
H13	H18	0.00050455288334
H14	H18	4.3742638847e-05
H15	H18	7.8006978369e-05
H16	H18	0.00030485638212
H17	H18	0.0061002854893
C1	H19	0.0088161703446
C2	H19	0.0007870528673
C3	H19	0.00052601265553
C4	H19	6.9247415085e-05
C5	H19	0.00010066385639
C6	H19	0.00031176867982
C7	H19	0.0010704352321
C8	H19	0.041028985268
C9	H19	0.9710329486
C1	H19	0.063559760055
C11	H19	0.010195112541
C12	H19	0.0039114026
H13	H19	4.3744307904e-05
H14	H19	4.0131986424e-06
H15	H19	7.7471060032e-06
H16	H19	8.145909332e-05
H17	H19	6.0625345174e-05
H18	H19	0.0054810594274
C1	C2	0.0036835212154
C2	C2	0.00072738189712
C3	C2	0.00052226833349



C4	C2	9.0345561876e-05
C5	C2	0.00011011518876
C6	C2	0.00042062406914
C7	C2	0.00039662918835
C8	C2	0.010148858732
C9	C2	0.063909308113
C1	C2	0.97293517445
C11	C2	0.040772150534
C12	C2	0.0087462359469
H13	C2	7.8005938121e-05
H14	C2	7.7472137568e-06
H15	C2	1.0794321699e-05
H16	C2	2.9542106506e-05
H17	C2	0.00010688112596
H18	C2	0.0012758800281
H19	C2	0.0089306573913
C1	H21	0.0012401073912
C2	H21	0.010273681408
C3	H21	0.0029141385882
C4	H21	0.00041007846151
C5	H21	0.00039239165592
C6	H21	0.00011825855993
C7	H21	0.0002123253266
C8	H21	0.00088788454193
C9	H21	0.008897817136
C1	H21	0.040574829908
C11	H21	0.96998200378
C12	H21	0.065432463493
H13	H21	0.00030486008192
H14	H21	8.1459157194e-05
H15	H21	2.9541760792e-05
H16	H21	8.1185883485e-06
H17	H21	4.0932517728e-05
H18	H21	9.9113924889e-05
H19	H21	0.0013359491477
C2	H21	0.0051477929372
C1	H22	0.0054577147068
C2	H22	0.039797325892
C3	H22	0.013604209998
C4	H22	0.00088145260455
C5	H22	0.0013777266113
C6	H22	0.00020586251717
C7	H22	0.00087034073071
C8	H22	0.0015558485308
C9	H22	0.0037227471551
C1	H22	0.010280600379
C11	H22	0.062936916516
C12	H22	0.96504633905

H13	H22	0.0060998930351
H14	H22	6.0625111083e-05
H15	H22	0.00010688017388
H16	H22	4.0932444148e-05
H17	H22	0.00013740384608
H18	H22	0.00015368213609
H19	H22	0.00035603485156
C2	H22	0.0013229072654
H21	H22	0.0089381479911

## (16)ANNULENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.7142170393
C1	C3	0.065977319201
C2	C3	1.0781737076
C1	C4	1.0936463925
C2	C4	0.067659860767
C3	C4	0.016496252175
C1	C5	0.00058491442958
C2	C5	0.0011506338743
C3	C5	0.019312225113
C4	C5	0.0008850048696
C1	C6	0.00090904430418
C2	C6	0.00065154749485
C3	C6	0.0089181865584
C4	C6	0.0003096612536
C5	C6	1.7124027552
C1	C7	0.00019839445723
C2	C7	0.00025854607966
C3	C7	0.00069314924953
C4	C7	0.0015094608398
C5	C7	0.07414914989
C6	C7	1.0906783119
C1	C8	0.0043367876967
C2	C8	0.0086018695845
C3	C8	0.0005371429412
C4	C8	0.055938026968
C5	C8	0.00061834316257
C6	C8	0.0011793398696
C7	C8	0.019454901738
C1	C9	0.0099618179053
C2	C9	0.0043120679133

C3	C9	0.00028591225464
C4	C9	0.067815377035
C5	C9	0.0010706230507
C6	C9	0.00050922873076
C7	C9	0.0075931514862
C8	C9	1.7203729606
C1	C1	0.067664287731
C2	C1	0.060633173861
C3	C1	0.004049396602
C4	C1	1.7137155581
C5	C1	0.00027249603672
C6	C1	0.00019972926653
C7	C1	0.0006559602346
C8	C1	0.067421795195
C9	C1	1.074068918
C1	C11	0.051444200552
C2	C11	0.06713254247
C3	C11	1.7214127791
C4	C11	0.0039293078448
C5	C11	0.013731949164
C6	C11	0.0037665870674
C7	C11	0.00030004273224
C8	C11	0.0012893066156
C9	C11	0.00052793105115
C1	C11	0.0072052248101
C1	C12	0.0038227605381
C2	C12	0.0096140632772
C3	C12	0.067194209303
C4	C12	0.00028911584342
C5	C12	0.065359219134
C6	C12	0.050046171767
C7	C12	0.0040367344259
C8	C12	0.00018130091902
C9	C12	0.00020556812767
C1	C12	0.00056181346942
C11	C12	1.0726449349
C1	C13	0.0065190141855
C2	C13	0.0035181750298
C3	C13	0.047837512261
C4	C13	0.00050484143196
C5	C13	1.0796644672
C6	C13	0.066501149435
C7	C13	0.009992419996
C8	C13	0.0002396440364
C9	C13	0.00015998118849
C1	C13	0.0011596790328
C11	C13	0.062291459712
C12	C13	1.7283035999

C1	C14	0.00024389137075
C2	C14	0.00023110102748
C3	C14	0.0016011252387
C4	C14	0.00061685306111
C5	C14	0.060273058565
C6	C14	0.067598465208
C7	C14	1.7169787516
C8	C14	0.016834843102
C9	C14	0.0044192796637
C1	C14	0.00032847724818
C11	C14	0.00063813157628
C12	C14	0.0090275290608
C13	C14	0.0046341784315
C1	C15	0.00062425534854
C2	C15	0.0018229971891
C3	C15	0.0002034793519
C4	C15	0.0074405632827
C5	C15	0.0041565333832
C6	C15	0.0096540515031
C7	C15	0.067228335553
C8	C15	0.065633619364
C9	C15	0.055188476622
C1	C15	0.0039964698429
C11	C15	0.00031182381596
C12	C15	0.00061198453032
C13	C15	0.00040796707109
C14	C15	1.0641811302
C1	C16	0.00033914831622
C2	C16	0.00067720050821
C3	C16	0.00021867025629
C4	C16	0.0040570666307
C5	C16	0.0057350889725
C6	C16	0.0032694230822
C7	C16	0.041855500661
C8	C16	1.0814500338
C9	C16	0.067795683025
C1	C16	0.0099552137337
C11	C16	0.00017666446267
C12	C16	0.0011367252706
C13	C16	0.00047509168211
C14	C16	0.063098102309
C15	C16	1.7309073747
C1	H17	0.96882301551
C2	H17	0.061297744597
C3	H17	0.0098704109129
C4	H17	0.039734379953
C5	H17	6.0565301058e-05
C6	H17	7.8002530356e-05

C7	H17	3.3812014787e-05
C8	H17	0.00045237122126
C9	H17	0.00067751857099
C1	H17	0.0081601273327
C11	H17	0.003572758604
C12	H17	0.0004246099104
C13	H17	0.00045588748996
C14	H17	1.9140215381e-05
C15	H17	4.2287314484e-05
C16	H17	5.8447260166e-05
C1	H18	0.061610753064
C2	H18	0.96969777315
C3	H18	0.039783383628
C4	H18	0.0098967465466
C5	H18	0.00031330168398
C6	H18	0.00027220113297
C7	H18	3.1819815415e-05
C8	H18	0.00058364309505
C9	H18	0.00045416187139
C1	H18	0.0042545150903
C11	H18	0.0094682639026
C12	H18	0.00071044075399
C13	H18	0.00042477434944
C14	H18	5.5087683543e-05
C15	H18	0.0001283854767
C16	H18	5.0447057373e-05
H17	H18	0.0078132786973
C1	H19	0.0075028342639
C2	H19	0.036797363464
C3	H19	0.93741154912
C4	H19	0.012426517089
C5	H19	0.020619312435
C6	H19	0.005765857106
C7	H19	0.00037950519464
C8	H19	0.00029837977147
C9	H19	0.00018294117387
C1	H19	0.001945680404
C11	H19	0.056769700997
C12	H19	0.010885665775
C13	H19	0.0082047230576
C14	H19	0.00043110057698
C15	H19	5.8339333958e-05
C16	H19	6.5887413649e-05
H17	H19	0.00044675018091
H18	H19	0.0070105552247
C1	C2	0.037080604208
C2	C2	0.0065395489004
C3	C2	0.016506260633

C4	C2	0.93772674642
C5	C2	0.0033272099133
C6	C2	0.0013086408403
C7	C2	0.0023892612974
C8	C2	0.016375142721
C9	C2	0.012750022838
C1	C2	0.058406297634
C11	C2	0.0025815259462
C12	C2	0.00023025106159
C13	C2	0.00052368298942
C14	C2	0.00041691935874
C15	C2	0.00037035698757
C16	C2	0.0010654317123
H17	C2	0.0081973649441
H18	C2	0.00036204426182
H19	C2	0.01813419486
C1	H21	0.00052991220035
C2	H21	0.0007843235655
C3	H21	0.019693876842
C4	H21	0.0020001192159
C5	H21	0.94208691618
C6	H21	0.056632117479
C7	H21	0.013614223645
C8	H21	0.00011375366653
C9	H21	9.7936637652e-05
C1	H21	0.00036263514194
C11	H21	0.013147331872
C12	H21	0.0081865436135
C13	H21	0.038085622879
C14	H21	0.0027743360251
C15	H21	0.00020212446039
C16	H21	0.00023184731871
H17	H21	9.1690865663e-05
H18	H21	0.00013153010233
H19	H21	0.008514709312
C2	H21	0.0046619800036
C1	H22	5.9015432953e-05
C2	H22	5.1595847071e-05
C3	H22	0.00069170031713
C4	H22	4.1494564119e-05
C5	H22	0.059343520424
C6	H22	0.96539434062
C7	H22	0.03900583112
C8	H22	0.00020885363923
C9	H22	0.0001015474164
C1	H22	1.9928535548e-05
C11	H22	0.00044029682035
C12	H22	0.0025167567397

C13	H22	0.0097072216729
C14	H22	0.0076936505349
C15	H22	0.00067743620796
C16	H22	0.00032651814888
H17	H22	5.14769474e-06
H18	H22	1.6446756412e-05
H19	H22	0.00024110635954
C2	H22	0.00017521727267
H21	H22	0.011304840977
C1	H23	0.00014701111383
C2	H23	4.9367272875e-05
C3	H23	8.7964477912e-05
C4	H23	0.0014520918304
C5	H23	0.011745981212
C6	H23	0.038967963502
C7	H23	0.94384989176
C8	H23	0.013916327118
C9	H23	0.0035874155045
C1	H23	0.0003637655769
C11	H23	4.3585658209e-05
C12	H23	0.00027059951859
C13	H23	0.00090059114967
C14	H23	0.055983382232
C15	H23	0.012431067157
C16	H23	0.0088014986565
H17	H23	5.6562115432e-05
H18	H23	3.8834138608e-06
H19	H23	7.2270770686e-05
C2	H23	0.00314625443
H21	H23	0.010305766593
H22	H23	0.0084863641513
C1	H24	0.00094549789877
C2	H24	0.00045506273943
C3	H24	0.00013491156105
C4	H24	0.014910023743
C5	H24	0.00070215028039
C6	H24	0.0016050491142
C7	H24	0.022775433548
C8	H24	0.93555890669
C9	H24	0.054797399898
C1	H24	0.011981762372
C11	H24	0.0001063835456
C12	H24	8.02022118e-05
C13	H24	6.239470705e-05
C14	H24	0.017741675661
C15	H24	0.0073581710276
C16	H24	0.037315475807
H17	H24	0.00024631642131



H18	H24	3.4442991602e-05
H19	H24	0.00028564954068
C2	H24	0.014965449772
H21	H24	9.4747189922e-05
H22	H24	7.9937426383e-05
H23	H24	0.0056526621634
C1	H25	0.0012533374986
C2	H25	0.00093398619959
C3	H25	5.8518997429e-05
C4	H25	0.0095872535112
C5	H25	7.67711116876e-05
C6	H25	5.3842122392e-05
C7	H25	0.00072131424018
C8	H25	0.062408667035
C9	H25	0.97002713419
C1	H25	0.040000756267
C11	H25	0.00013139661858
C12	H25	2.1249076219e-05
C13	H25	2.4304791497e-05
C14	H25	0.00057377916401
C15	H25	0.0028866374296
C16	H25	0.009995870634
H17	H25	3.4503559325e-05
H18	H25	9.967310971e-05
H19	H25	3.5977781423e-05
C2	H25	0.00084063637959
H21	H25	8.3997228004e-06
H22	H25	6.1105660275e-06
H23	H25	0.00016448804483
H24	H25	0.011347065537
C1	H26	0.009423331859
C2	H26	0.0030799149726
C3	H26	0.00050399405764
C4	H26	0.061877951806
C5	H26	5.0038320082e-05
C6	H26	2.5714833638e-05
C7	H26	0.00017910473855
C8	H26	0.0087388462026
C9	H26	0.038854420744
C1	H26	0.97053723969
C11	H26	0.00044265430248
C12	H26	3.7472151848e-05
C13	H26	6.8255252168e-05
C14	H26	7.7373392017e-05
C15	H26	0.00084242982374
C16	H26	0.0012251681938
H17	H26	0.0054583362876
H18	H26	0.00020750332956

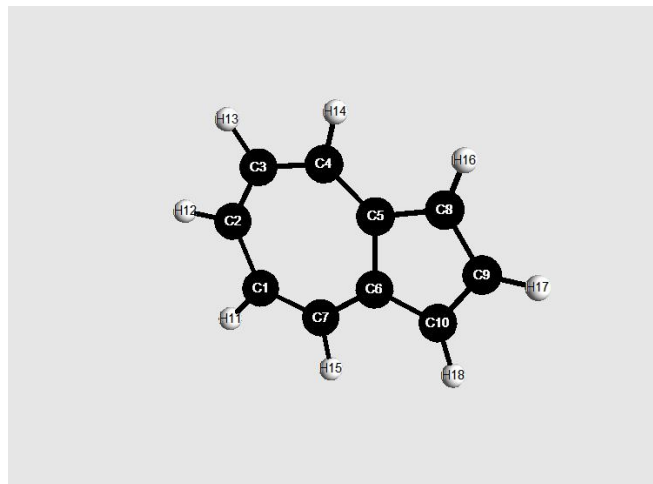
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C2	H26	0.011265850621
H21	H26	0.00011037025138
H22	H26	4.2187290691e-06
H23	H26	0.000123184572
H24	H26	0.0007287215181
H25	H26	0.0035065518108
C1	H27	0.0027255307147
C2	H27	0.010352399916
C3	H27	0.062081111285
C4	H27	0.00044038380364
C5	H27	0.00084162070108
C6	H27	0.0010646300391
C7	H27	7.7193452585e-05
C8	H27	7.8666370286e-05
C9	H27	3.6744807373e-05
C1	H27	0.00042517158977
C11	H27	0.96823567068
C12	H27	0.040059108295
C13	H27	0.0097957563076
C14	H27	0.00021246952299
C15	H27	2.9820525932e-05
C16	H27	3.2824071821e-05
H17	H27	0.00019409054709
H18	H27	0.0050741453386
H19	H27	0.011379885882
C2	H27	0.00034787542461
H21	H27	0.00039800846226
H22	H27	5.5568186459e-05
H23	H27	3.9545619037e-06
H24	H27	1.1470295567e-05
H25	H27	7.0957488053e-06
H26	H27	3.2288052987e-05
C1	H28	0.0010861608158
C2	H28	0.0013071349799
C3	H28	0.010591177435
C4	H28	7.4153052043e-05
C5	H28	0.010122773242
C6	H28	0.0036876869662
C7	H28	0.00043687365869
C8	H28	4.0475734069e-05
C9	H28	2.6457894412e-05
C1	H28	0.00019552632011
C11	H28	0.040478074951
C12	H28	0.97112205456
C13	H28	0.064902191309
C14	H28	0.00064109029666
C15	H28	5.3095739876e-05

C16	H28	8.0693219236e-05
H17	H28	9.5857251024e-05
H18	H28	8.5729472499e-05
H19	H28	0.00061231124146
C2	H28	2.9082788244e-05
H21	H28	0.00046434817105
H22	H28	0.00018704237089
H23	H28	2.5459478897e-05
H24	H28	7.2872225924e-06
H25	H28	4.5629236584e-06
H26	H28	1.0852853588e-05
H27	H28	0.0037349434032
C1	H29	0.00044740382629
C2	H29	0.00029328413297
C3	H29	0.003026240156
C4	H29	5.3506718968e-05
C5	H29	0.039959434656
C6	H29	0.0094636016386
C7	H29	0.0008078504955
C8	H29	2.5977587294e-05
C9	H29	2.3733792001e-05
C1	H29	7.9766340804e-05
C11	H29	0.009978554657
C12	H29	0.063354391032
C13	H29	0.96743419584
C14	H29	0.00074351374784
C15	H29	5.4366026635e-05
C16	H29	8.1240058661e-05
H17	H29	3.0694088107e-05
H18	H29	4.3130418917e-05
H19	H29	0.00039112090985
C2	H29	0.00011457924554
H21	H29	0.0072853045098
H22	H29	0.0045318677441
H23	H29	0.00026399805803
H24	H29	9.5455857721e-06
H25	H29	2.5623876673e-06
H26	H29	5.0959648406e-06
H27	H29	0.0012094871524
H28	H29	0.0088121480156
C1	C3	2.7633073657e-05
C2	C3	5.6071296503e-05
C3	C3	8.6909056751e-05
C4	C3	0.00021692293318
C5	C3	0.0031830475016
C6	C3	0.010105054722
C7	C3	0.062370489891
C8	C3	0.00099408655654

C9	C3	0.0014093275303
C1	C3	9.6506714879e-05
C11	C3	4.2567244799e-05
C12	C3	0.00043780701833
C13	C3	0.00021354661776
C14	C3	0.96814931903
C15	C3	0.03984387373
C16	C3	0.011598775928
H17	C3	2.8854397154e-06
H18	C3	5.7929151911e-06
H19	C3	2.1701071645e-05
C2	C3	8.2923148211e-05
H21	C3	0.00044810114364
H22	C3	0.005800654452
H23	C3	0.011623360074
H24	C3	0.00047805286747
H25	C3	8.2335732044e-05
H26	C3	2.731519686e-05
H27	C3	1.1230852104e-05
H28	C3	2.8704666141e-05
H29	C3	4.8678333189e-05
C1	H31	4.8581051269e-05
C2	H31	0.00013673205904
C3	H31	4.9569260346e-05
C4	H31	0.00053280092963
C5	H31	0.0015687552477
C6	H31	0.0013556827601
C7	H31	0.011705519093
C8	H31	0.0099901992534
C9	H31	0.0040049967574
C1	H31	0.00045447739025
C11	H31	3.5541586284e-05
C12	H31	0.00024803138151
C13	H31	0.00011928487526
C14	H31	0.040030591149
C15	H31	0.97174465074
C16	H31	0.064400435566
H17	H31	4.2821244113e-06
H18	H31	1.0521950642e-05
H19	H31	1.3833505003e-05
C2	H31	3.081281555e-05
H21	H31	6.190878137e-05
H22	H31	4.083586199e-05
H23	H31	0.00069224492732
H24	H31	0.0004169022441
H25	H31	0.00020953916829
H26	H31	9.5804213476e-05
H27	H31	7.2654275068e-06

H28	H31	1.9166645644e-05
H29	H31	2.1542228418e-05
C3	H31	0.0026048587152
C1	H32	6.7012387414e-05
C2	H32	6.5516599818e-05
C3	H32	1.8598790475e-05
C4	H32	0.00054432978084
C5	H32	0.00043088207842
C6	H32	0.00031931858
C7	H32	0.0027538005138
C8	H32	0.039616184846
C9	H32	0.0089967241963
C1	H32	0.00070273656287
C11	H32	1.3286167178e-05
C12	H32	8.7038022293e-05
C13	H32	3.6872731397e-05
C14	H32	0.010002537235
C15	H32	0.062899824708
C16	H32	0.96784729424
H17	H32	6.0081650449e-06
H18	H32	5.8104437039e-06
H19	H32	9.9951909229e-06
C2	H32	0.00029209876259
H21	H32	1.5788477969e-05
H22	H32	3.7891670505e-05
H23	H32	0.00037709932752
H24	H32	0.0076403520083
H25	H32	0.0052633187077
H26	H32	4.4133777687e-05
H27	H32	2.5460304642e-06
H28	H32	5.8160617698e-06
H29	H32	5.6638021342e-06
C3	H32	0.0012713647346
H31	H32	0.0083667121494

## AZULENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.2216269626
C1	C3	0.062556426733
C2	C3	1.5411801858
C1	C4	0.031733653362
C2	C4	0.071168828762
C3	C4	1.2230878803
C1	C5	0.011226283639
C2	C5	0.057543270114
C3	C5	0.059776773726
C4	C5	1.5057236313
C1	C6	0.06035787148
C2	C6	0.028919014474
C3	C6	0.011045411761
C4	C6	0.074777978158
C5	C6	1.0396626791
C1	C7	1.5410687194
C2	C7	0.070440949922
C3	C7	0.062661588439
C4	C7	0.014960458732
C5	C7	0.065585216089
C6	C7	1.2128042146
C1	C8	0.025170385957
C2	C8	0.007224861235
C3	C8	0.029618322969
C4	C8	0.071602468193
C5	C8	1.1822432976
C6	C8	0.10652799529
C7	C8	0.01658243619
C1	C9	0.0082533623174
C2	C9	0.023830571637

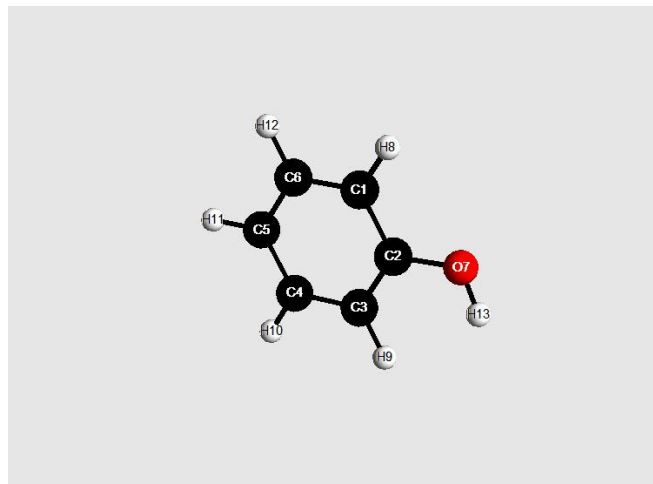
C3	C9	0.0079324365472
C4	C9	0.05982061775
C5	C9	0.084318877725
C6	C9	0.082757071486
C7	C9	0.03094639224
C8	C9	1.5295531825
C1	C1	0.05849870575
C2	C1	0.01020802404
C3	C1	0.023332458591
C4	C1	0.035964587009
C5	C1	0.085757038356
C6	C1	1.477514497
C7	C1	0.067018577103
C8	C1	0.085030180655
C9	C1	1.2163452057
C1	H11	0.97319035321
C2	H11	0.046345306655
C3	H11	0.0079083880544
C4	H11	0.0018786371502
C5	H11	0.00052433163696
C6	H11	0.0092941842208
C7	H11	0.058970148452
C8	H11	0.0019662438692
C9	H11	0.00061296357034
C1	H11	0.0044180097969
C1	H12	0.044413278958
C2	H12	0.96772294423
C3	H12	0.057311659092
C4	H12	0.0094518237195
C5	H12	0.0035646002932
C6	H12	0.0016564601123
C7	H12	0.0077957762616
C8	H12	0.00043335461614
C9	H12	0.0016059024139
C1	H12	0.00065371712747
H11	H12	0.0075135385349
C1	H13	0.0094271976588
C2	H13	0.058644649976
C3	H13	0.972578555
C4	H13	0.046164953502
C5	H13	0.0076193825861
C6	H13	0.00053924507067
C7	H13	0.0039888670282
C8	H13	0.0024522551804
C9	H13	0.00046338950838
C1	H13	0.0018514976267
H11	H13	0.0011540693788
H12	H13	0.0091233999926

C1	H14	0.0014752374372
C2	H14	0.0075647150982
C3	H14	0.042605775761
C4	H14	0.96165441393
C5	H14	0.054184976874
C6	H14	0.010294491712
C7	H14	0.00069658212938
C8	H14	0.012203761535
C9	H14	0.0030060149211
C1	H14	0.0029575013969
H11	H14	0.00013671168811
H12	H14	0.0011433418648
H13	H14	0.0070973267301
C1	H15	0.053929078543
C2	H15	0.0090905316383
C3	H15	0.0032773291062
C4	H15	0.00078588630319
C5	H15	0.0092395418938
C6	H15	0.043896295659
C7	H15	0.9610563803
C8	H15	0.0016736090939
C9	H15	0.001709845945
C1	H15	0.010535107688
H11	H15	0.0087727572842
H12	H15	0.0011339798516
H13	H15	0.0002991667184
H14	H15	0.00016003846069
C1	H16	0.0018221126604
C2	H16	0.00037595752535
C3	H16	0.0016423436936
C4	H16	0.0061718642348
C5	H16	0.041847370252
C6	H16	0.012066381576
C7	H16	0.0017407653015
C8	H16	0.98391012904
C9	H16	0.050866024362
C1	H16	0.010620769919
H11	H16	0.00013775478915
H12	H16	3.0667300214e-05
H13	H16	0.00012207577252
H14	H16	0.0051592788957
H15	H16	0.00041924625811
C1	H17	0.00054622615389
C2	H17	0.001510906699
C3	H17	0.00059726259283
C4	H17	0.0043235000426
C5	H17	0.0097451150176
C6	H17	0.0080698310352



C7	H17	0.0025112330379
C8	H17	0.051912617801
C9	H17	0.982769331
C1	H17	0.040142059414
H11	H17	7.9511968486e-05
H12	H17	9.7318808841e-05
H13	H17	7.5317559379e-05
H14	H17	0.00018276966143
H15	H17	8.8390840081e-05
H16	H17	0.0036733512583
C1	H18	0.0032297707424
C2	H18	0.00069717591357
C3	H18	0.0016370372827
C4	H18	0.0028876926313
C5	H18	0.011049674886
C6	H18	0.052762972706
C7	H18	0.0068634721524
C8	H18	0.0088299800154
C9	H18	0.040082634578
C1	H18	0.98503479745
H11	H18	0.00023311926581
H12	H18	5.1811296408e-05
H13	H18	0.00012564955508
H14	H18	0.00050406736633
H15	H18	0.005096858861
H16	H18	0.0015421754798
H17	H18	0.0025459041952

## PHENOL



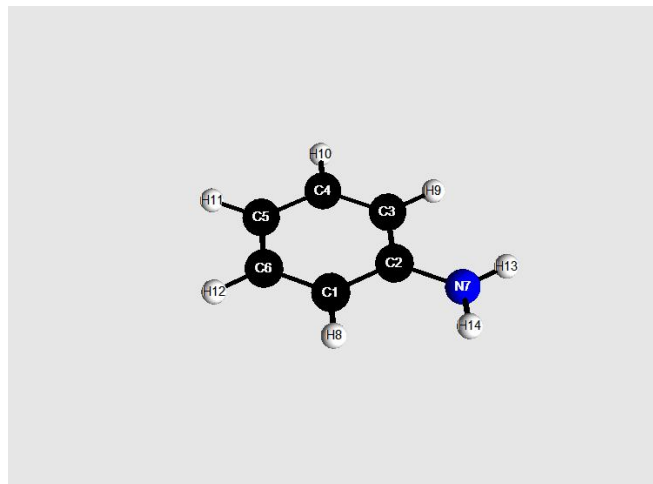
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3006053106
C1	C3	0.064437262545
C2	C3	1.3238226216
C1	C4	0.096746679705
C2	C4	0.073982016181
C3	C4	1.37948224
C1	C5	0.07169802364
C2	C5	0.086201077554
C3	C5	0.07307851911
C4	C5	1.3965687842
C1	C6	1.4027778563
C2	C6	0.0769094158
C3	C6	0.095230504032
C4	C6	0.078170695556
C5	C6	1.3736325488
C1	O7	0.10871468292
C2	O7	0.82934322519
C3	O7	0.11548893636
C4	O7	0.014763765228
C5	O7	0.019291838686
C6	O7	0.013497668925
C1	H8	0.96929978243
C2	H8	0.046653202322
C3	H8	0.0067760136553
C4	H8	0.0058621543836
C5	H8	0.0083397498972
C6	H8	0.046748256288
O7	H8	0.015582832022
C1	H9	0.0071954946387
C2	H9	0.050183852254

C3	H9	0.97519725986
C4	H9	0.048215091098
C5	H9	0.0086286267616
C6	H9	0.0063842734218
O7	H9	0.016062954566
H8	H9	0.0016812343305
C1	C1	0.0061675146528
C2	C1	0.0083680207048
C3	C1	0.049309753527
C4	C1	0.97476407272
C5	C1	0.048387115805
C6	C1	0.0088123846044
O7	C1	0.0017518035468
H8	C1	0.00036136299683
H9	C1	0.0059254862402
C1	H11	0.0087407222452
C2	H11	0.0057242628328
C3	H11	0.0089950014374
C4	H11	0.050559949753
C5	H11	0.97978547576
C6	H11	0.049344031079
O7	H11	0.0015405403634
H8	H11	0.0012877352499
H9	H11	0.0013352055903
C1	H11	0.0056382323041
C1	H12	0.049791724847
C2	H12	0.0085122450623
C3	H12	0.0060086964215
C4	H12	0.008711461752
C5	H12	0.047727469821
C6	H12	0.9745729193
O7	H12	0.001444100565
H8	H12	0.0057919646987
H9	H12	0.00039424106661
C1	H12	0.0014742851302
H11	H12	0.0055263722898
C1	H13	0.0055910310317
C2	H13	0.010171815601
C3	H13	0.0049647361614
C4	H13	0.00041755850127
C5	H13	0.00026019500977
C6	H13	0.00095140092869
O7	H13	0.57911618568
H8	H13	0.00035998234989
H9	H13	0.0039674536816
C1	H13	4.3765394718e-05
H11	H13	5.2595792411e-05
H12	H13	0.00020049243603



## ANILINE



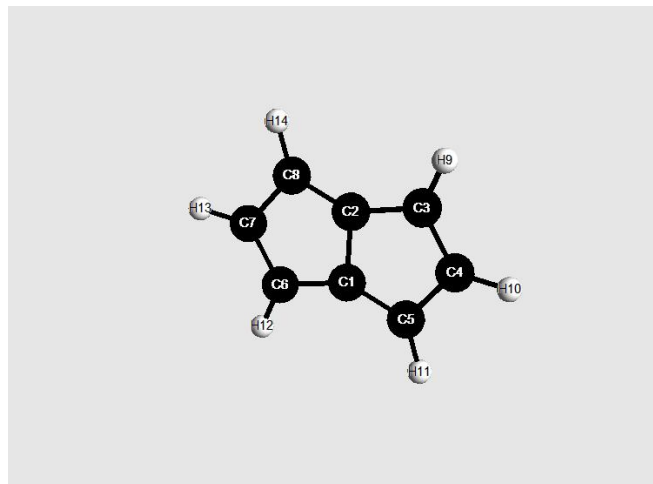
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.2952986653
C1	C3	0.065303257066
C2	C3	1.2952999924
C1	C4	0.092949816399
C2	C4	0.073122099543
C3	C4	1.4017559455
C1	C5	0.07271454065
C2	C5	0.082599148321
C3	C5	0.072731493175
C4	C5	1.3800595779
C1	C6	1.4017381096
C2	C6	0.073116392865
C3	C6	0.09295132385
C4	C6	0.07869441628
C5	C6	1.3800977204
C1	N7	0.1084882333
C2	N7	0.976983225
C3	N7	0.10846501312
C4	N7	0.014844311058
C5	N7	0.024743152775
C6	N7	0.014843573617
C1	H8	0.9768451972
C2	H8	0.048583313556
C3	H8	0.0073815124835
C4	H8	0.0061349558223
C5	H8	0.0087500823304
C6	H8	0.05009339187
N7	H8	0.014637980662
C1	H9	0.0073797246096
C2	H9	0.048568481352

C3	H9	0.97687505381
C4	H9	0.050072683875
C5	H9	0.0087506956306
C6	H9	0.0061333678651
N7	H9	0.014635149151
H8	H9	0.0017402641145
C1	C1	0.0060894089794
C2	C1	0.0084955771952
C3	C1	0.050363031305
C4	C1	0.97516497518
C5	C1	0.048228645623
C6	C1	0.0088839011368
N7	C1	0.0014712847571
H8	C1	0.00039764759448
H9	C1	0.0061618544582
C1	H11	0.0091238529413
C2	H11	0.0056332116943
C3	H11	0.0091246671125
C4	H11	0.050382085215
C5	H11	0.98281956164
C6	H11	0.050383258111
N7	H11	0.0021641908569
H8	H11	0.0013580446856
H9	H11	0.0013580408107
C1	H11	0.005605014331
C1	H12	0.050344021979
C2	H12	0.0084957581131
C3	H12	0.0060908397201
C4	H12	0.0088852620324
C5	H12	0.04824344977
C6	H12	0.97524503221
N7	H12	0.0014712804506
H8	H12	0.0061618639261
H9	H12	0.00039764380006
C1	H12	0.0014914096105
H11	H12	0.0056050071256
C1	H13	0.007495260437
C2	H13	0.017707670842
C3	H13	0.0057148915638
C4	H13	0.00049910131076
C5	H13	0.00078016738373
C6	H13	0.00131130433
N7	H13	0.82399447613
H8	H13	0.00056175098755
H9	H13	0.0042885728813
C1	H13	3.8282886724e-05
H11	H13	8.9307913463e-05
H12	H13	0.00025223443687

C1	H14	0.0057206267945
C2	H14	0.017710246807
C3	H14	0.0074937305488
C4	H14	0.001311332089
C5	H14	0.00078015595879
C6	H14	0.0004990931102
N7	H14	0.82399672054
H8	H14	0.0042885382439
H9	H14	0.00056174129037
C1	H14	0.00025223547235
H11	H14	8.9307859509e-05
H12	H14	3.8282800855e-05
H13	H14	0.016516940481

## PENTALENE



### HARTREE-FOCK

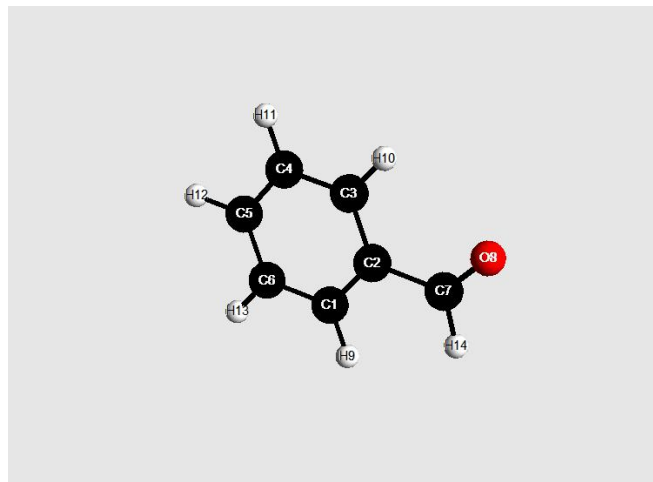
Atom A	Atom B	Delocalization index
C1	C2	1.0266265125
C1	C3	0.093012733295
C2	C3	1.0483057244
C1	C4	0.076168435744
C2	C4	0.085503771648
C3	C4	1.7378493601
C1	C5	1.6854960283
C2	C5	0.081514078035
C3	C5	0.075018237934
C4	C5	1.0380639499
C1	C6	1.0483052597
C2	C6	0.093013173772
C3	C6	0.014315546155
C4	C6	0.014288315397
C5	C6	0.059661224092
C1	C7	0.085503241691
C2	C7	0.076168679253
C3	C7	0.014288266565
C4	C7	0.0080240914234
C5	C7	0.054318437714
C6	C7	1.7378493037
C1	C8	0.081513360606
C2	C8	1.6854958443
C3	C8	0.059661248687
C4	C8	0.054318537239
C5	C8	0.062186436204
C6	C8	0.075018348344
C7	C8	1.0380641948
C1	H9	0.011235964459
C2	H9	0.035200278662



C3	H9	0.98105277427
C4	H9	0.058512119134
C5	H9	0.010589239377
C6	H9	0.001288378393
C7	H9	0.00085908542338
C8	H9	0.0020693931434
C1	C1	0.0068279722875
C2	C1	0.01083355497
C3	C1	0.060190600706
C4	C1	0.98356228582
C5	C1	0.035805265832
C6	C1	0.0019103743411
C7	C1	0.00086140119051
C8	C1	0.0041947391583
H9	C1	0.0041870209476
C1	H11	0.056587065108
C2	H11	0.010616808346
C3	H11	0.0065272519546
C4	H11	0.034729835757
C5	H11	0.9808195152
C6	H11	0.003536422118
C7	H11	0.0024280760171
C8	H11	0.0042397157384
H9	H11	0.001304859827
C1	H11	0.0017495141151
C1	H12	0.035200201807
C2	H12	0.011235950719
C3	H12	0.0012883749682
C4	H12	0.00085908666133
C5	H12	0.0020693840621
C6	H12	0.98105299285
C7	H12	0.058511858946
C8	H12	0.010589216705
H9	H12	0.0003296185547
C1	H12	8.332967247e-05
H11	H12	0.00053482000674
C1	H13	0.010833469319
C2	H13	0.0068279462122
C3	H13	0.0019103526282
C4	H13	0.00086139646651
C5	H13	0.0041947139226
C6	H13	0.060190174872
C7	H13	0.9835602622
C8	H13	0.035805057818
H9	H13	8.3328437088e-05
C1	H13	0.00023781307838
H11	H13	0.00013930434016
H12	H13	0.0041868851874

C1	H14	0.010616781532
C2	H14	0.056586994008
C3	H14	0.0035364331326
C4	H14	0.0024280750332
C5	H14	0.004239706505
C6	H14	0.0065272630805
C7	H14	0.034729819269
C8	H14	0.98081948537
H9	H14	0.00053482335639
C1	H14	0.00013930555635
H11	H14	0.00063784349031
H12	H14	0.0013048610115
H13	H14	0.0017495075806

## BENZALDEHYDE



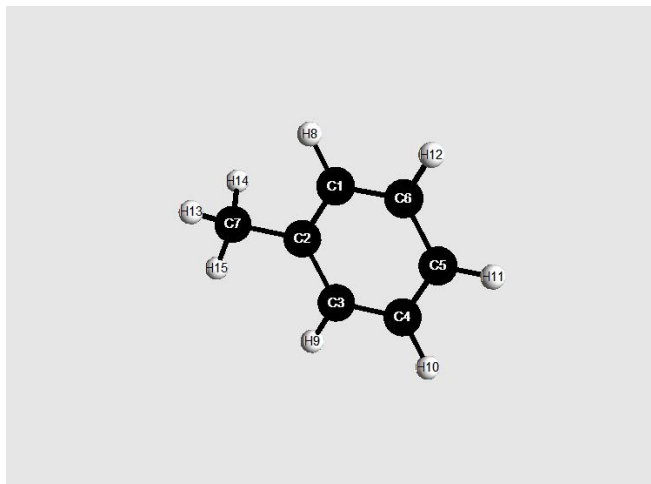
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3690686323
C1	C3	0.069928724944
C2	C3	1.3313541498
C1	C4	0.093817209842
C2	C4	0.073501305237
C3	C4	1.4130392497
C1	C5	0.077219598493
C2	C5	0.092364324459
C3	C5	0.076355717207
C4	C5	1.3644105537
C1	C6	1.3778589218
C2	C6	0.070590566381
C3	C6	0.096129243369
C4	C6	0.07192980312
C5	C6	1.3983771292
C1	C7	0.06259199175
C2	C7	0.98074934909
C3	C7	0.049371520799
C4	C7	0.0086620330179
C5	C7	0.01048018115
C6	C7	0.008056151316
C1	O8	0.028373248631
C2	O8	0.12236990185
C3	O8	0.04050910227
C4	O8	0.003789656237
C5	O8	0.011795703355
C6	O8	0.003997102119
C7	O8	1.2966017834
C1	H9	0.96765930138
C2	H9	0.04697535879

C3	H9	0.0085423629423
C4	H9	0.0059108356389
C5	H9	0.0083186553286
C6	H9	0.04701856388
C7	H9	0.010768504266
O8	H9	0.002900779021
C1	C1	0.0079212228429
C2	C1	0.041734784155
C3	C1	0.95522716178
C4	C1	0.045066966704
C5	C1	0.0078795778852
C6	C1	0.0051313314806
C7	C1	0.0050334571537
O8	C1	0.023550466213
H9	C1	0.0014308416252
C1	H11	0.0056832256361
C2	H11	0.0086254961235
C3	H11	0.0496803982
C4	H11	0.97476171064
C5	H11	0.048022220876
C6	H11	0.0083020852681
C7	H11	0.0011738898665
O8	H11	0.00020690725399
H9	H11	0.00038753946892
C1	H11	0.0053533574784
C1	H12	0.0085664836678
C2	H12	0.005582920508
C3	H12	0.008311829152
C4	H12	0.047135183151
C5	H12	0.97372700036
C6	H12	0.048604540919
C7	H12	0.00057286608685
O8	H12	0.00081078933437
H9	H12	0.0013135256338
C1	H12	0.0012213172382
H11	H12	0.005439747028
C1	H13	0.048823715962
C2	H13	0.008483475476
C3	H13	0.0059101572897
C4	H13	0.0084593682815
C5	H13	0.049128451917
C6	H13	0.97550461296
C7	H13	0.0010614996408
O8	H13	0.00056311914093
H9	H13	0.0054616358723
C1	H13	0.00033781004207
H11	H13	0.0013181602781
H12	H13	0.005572382801

C1	H14	0.012021914255
C2	H14	0.049656709548
C3	H14	0.0066650243986
C4	H14	0.0016200789752
C5	H14	0.00072743979344
C6	H14	0.0010067380787
C7	H14	0.88448220849
O8	H14	0.12041478142
H9	H14	0.011571024673
C1	H14	0.00077117596089
H11	H14	0.00042277393244
H12	H14	6.8900731616e-05
H13	H14	2.9292518917e-05

## TOLUENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3529709674
C1	C3	0.074347839685
C2	C3	1.3780029372
C1	C4	0.099141830083
C2	C4	0.072271131561
C3	C4	1.3765924632
C1	C5	0.073024852801
C2	C5	0.094437768576
C3	C5	0.073300603401
C4	C5	1.3988068447
C1	C6	1.4016152859
C2	C6	0.072408090525
C3	C6	0.097048440771
C4	C6	0.07581786824
C5	C6	1.3753741559
C1	C7	0.05003912168
C2	C7	1.0006553397
C3	C7	0.050073047955
C4	C7	0.0078709759638
C5	C7	0.0049625174695
C6	C7	0.0083077724305
C1	H8	0.97318822784
C2	H8	0.047295827167
C3	H8	0.0084387983805
C4	H8	0.0062369060885
C5	H8	0.0085461161991
C6	H8	0.050631452494
C7	H8	0.010338262832
C1	H9	0.0084665347406
C2	H9	0.048430567038

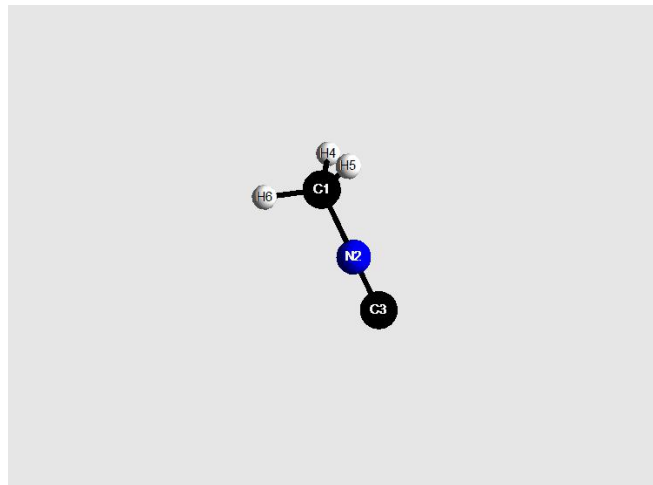
C3	H9	0.97190209073
C4	H9	0.049376736571
C5	H9	0.0084890389254
C6	H9	0.0062278275306
C7	H9	0.010698947754
H8	H9	0.0015842182872
C1	C1	0.0063860299062
C2	C1	0.0084990661368
C3	C1	0.049064932317
C4	C1	0.97698237879
C5	C1	0.049707611808
C6	C1	0.0087916251504
C7	C1	0.0011538094032
H8	C1	0.00041342414399
H9	C1	0.0058570314029
C1	H11	0.0086298606701
C2	H11	0.0061112365945
C3	H11	0.0087563962752
C4	H11	0.050065866207
C5	H11	0.97853042825
C6	H11	0.049137776731
C7	H11	0.00039206574832
H8	H11	0.0013633969958
H9	H11	0.0013519007358
C1	H11	0.0056867912702
C1	H12	0.05008088156
C2	H12	0.0086073221898
C3	H12	0.0062631429103
C4	H12	0.0086852166877
C5	H12	0.048764494992
C6	H12	0.97693549785
C7	H12	0.0011628725002
H8	H12	0.0059836672948
H9	H12	0.00041460347473
C1	H12	0.0014345009056
H11	H12	0.0055706040975
C1	H13	0.010268715753
C2	H13	0.045070648348
C3	H13	0.0098713732938
C4	H13	0.0015152498243
C5	H13	0.0033796156289
C6	H13	0.001092511516
C7	H13	0.95939887822
H8	H13	0.0028391241684
H9	H13	0.0007745283432
C1	H13	0.00017011460453
H11	H13	0.00024954403973
H12	H13	5.5794013809e-05

C1	H14	0.010271165403
C2	H14	0.045008384433
C3	H14	0.0098671517922
C4	H14	0.0015157914606
C5	H14	0.0033712621897
C6	H14	0.0010919250889
C7	H14	0.95936053468
H8	H14	0.0028574990327
H9	H14	0.00077581272819
C1	H14	0.00017053790731
H11	H14	0.00024901646661
H12	H14	5.5758968558e-05
H13	H14	0.042440037773
C1	H15	0.0079491894677
C2	H15	0.041752101795
C3	H15	0.012693348794
C4	H15	0.001060226578
C5	H15	0.00042606162082
C6	H15	0.0016062359057
C7	H15	0.96055737592
H8	H15	0.0011298422813
H9	H15	0.010411521686
C1	H15	7.8577476862e-05
H11	H15	6.3916548358e-05
H12	H15	0.00029943937809
H13	H15	0.041803505963
H14	H15	0.041802709725



# CYANIDES AND ISOCYANIDES

## ISOACETONITRILE



### HARTREE-FOCK

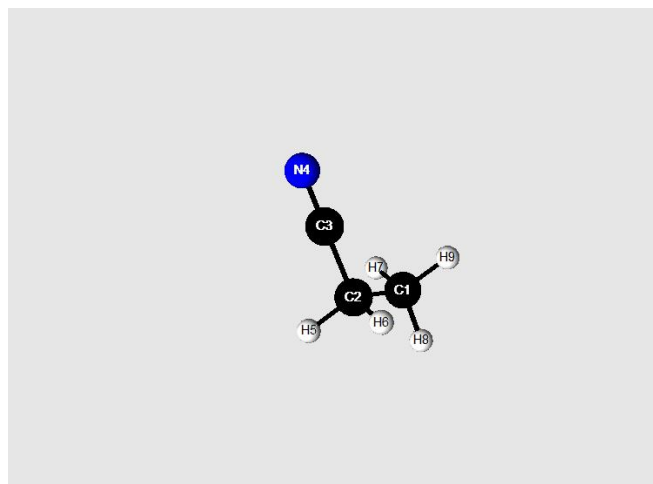
Atom A	Atom B	Delocalization index
C1	N2	0.83107107324
C1	C3	0.031809056057
N2	C3	1.7820915337
C1	H4	0.92735707307
N2	H4	0.075811275014
C3	H4	0.013388780145
C1	H5	0.92726777452
N2	H5	0.075819393776
C3	H5	0.013390755538
H4	H5	0.034615572686
C1	H6	0.92722873051
N2	H6	0.075831015944
C3	H6	0.013392405808
H4	H6	0.034617806773
H5	H6	0.034618083859

### CCSD

Atom A	Atom B	Delocalization index
C1	N2	0.7882517435
C1	C3	0.029420741329
N2	C3	1.5895480912
C1	H4	0.80257169033
N2	H4	0.054716273922
C3	H4	0.011003281602
C1	H5	0.8024676274
N2	H5	0.054720157383
C3	H5	0.011003821636
H4	H5	0.027561868065

C1	H6	0.8024320645
N2	H6	0.054725039944
C3	H6	0.01100354347
H4	H6	0.027558346221
H5	H6	0.027558079074

## PROPANENITRILE



## HARTREE-FOCK

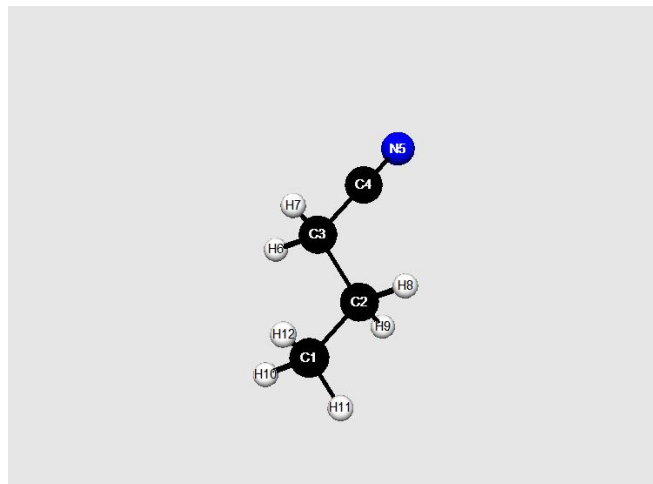
Atom A	Atom B	Delocalization index
C1	C2	0.96878491169
C1	C3	0.056613137602
C2	C3	0.97992806139
C1	N4	0.023161729482
C2	N4	0.08246162212
C3	N4	2.2298842966
C1	H5	0.035615085445
C2	H5	0.93598646725
C3	H5	0.054485148391
N4	H5	0.021301648812
C1	H6	0.035607224778
C2	H6	0.9359095662
C3	H6	0.054485972795
N4	H6	0.021301806633
H5	H6	0.03531237278
C1	H7	0.96218047009
C2	H7	0.043378422479
C3	H7	0.0069259698613
N4	H7	0.0034089490266
H5	H7	0.0031646499012
H6	H7	0.010382325729
C1	H8	0.96476918929
C2	H8	0.043925471453
C3	H8	0.01052166736
N4	H8	0.0038089100106
H5	H8	0.0034244127061
H6	H8	0.0034248681676
H7	H8	0.04035487347
C1	H9	0.962151414
C2	H9	0.043382647777

C3	H9	0.006923326166
N4	H9	0.003409369349
H5	H9	0.010382293115
H6	H9	0.0031643279046
H7	H9	0.040315726644
H8	H9	0.040354729758

#### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.83405495866
C1	C3	0.046897768243
C2	C3	0.87323514137
C1	N4	0.017045823839
C2	N4	0.060063785121
C3	N4	1.9131874492
C1	H5	0.029651833235
C2	H5	0.80515817218
C3	H5	0.041078918009
N4	H5	0.015392907965
C1	H6	0.029652193272
C2	H6	0.80500792355
C3	H6	0.041077939909
N4	H6	0.015392955088
H5	H6	0.028448329868
C1	H7	0.82708038324
C2	H7	0.034086851927
C3	H7	0.0072134350689
N4	H7	0.0026757376265
H5	H7	0.0027947596784
H6	H7	0.0083925467844
C1	H8	0.82959334201
C2	H8	0.034532148779
C3	H8	0.0079400859076
N4	H8	0.0030357724517
H5	H8	0.0030343624042
H6	H8	0.0030345202326
H7	H8	0.03162492564
C1	H9	0.8270823704
C2	H9	0.03409407958
C3	H9	0.0072119880538
N4	H9	0.0026763631148
H5	H9	0.0083927015958
H6	H9	0.0027956725991
H7	H9	0.031691272528
H8	H9	0.031624645148

## BUTANENITRILE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.98121301622
C1	C3	0.047194952474
C2	C3	0.95180361078
C1	C4	0.0097115797684
C2	C4	0.054776994357
C3	C4	0.97970639891
C1	N5	0.0035050341746
C2	N5	0.022378019333
C3	N5	0.082142202091
C4	N5	2.2284172898
C1	H6	0.0071667260875
C2	H6	0.033832037692
C3	H6	0.93224653079
C4	H6	0.054346408605
N5	H6	0.02107939308
C1	H7	0.0071714607186
C2	H7	0.033794734805
C3	H7	0.93225892915
C4	H7	0.054346739892
N5	H7	0.021079853302
H6	H7	0.035511925346
C1	H8	0.040457975601
C2	H8	0.94868894229
C3	H8	0.044006161743
C4	H8	0.0076017114694
N5	H8	0.0038874778068
H6	H8	0.010137113322
H7	H8	0.0031909565561
C1	H9	0.040454872377
C2	H9	0.94849621241

C3	H9	0.044003311503
C4	H9	0.0076068981548
N5	H9	0.0038894785132
H6	H9	0.0031886650626
H7	H9	0.01013719264
H8	H9	0.04024802478
C1	C1	0.96287201235
C2	C1	0.042242312819
C3	C1	0.0072796340882
C4	C1	0.00073641208758
N5	C1	0.00042986425941
H6	C1	0.0057628718667
H7	C1	0.00046498479996
H8	C1	0.011152008071
H9	C1	0.0034788343256
C1	H11	0.96462143068
C2	H11	0.042098088871
C3	H11	0.010498555007
C4	H11	0.0019640407478
N5	H11	0.00075611971584
H6	H11	0.00077978929183
H7	H11	0.00077895874005
H8	H11	0.0035826452064
H9	H11	0.0035800750784
C1	H11	0.042483005756
C1	H12	0.96288908184
C2	H12	0.042206272119
C3	H12	0.0072782083312
C4	H12	0.0007370625433
N5	H12	0.00042989390239
H6	H12	0.00046541446625
H7	H12	0.0057630436985
H8	H12	0.0034754648277
H9	H12	0.01115237279
C1	H12	0.043496466139
H11	H12	0.042483128419

#### CCSD

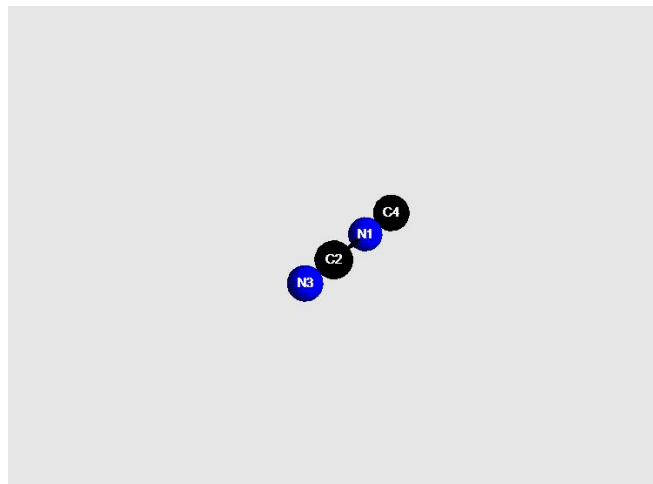
Atom A	Atom B	Delocalization index
C1	C2	0.84367382433
C1	C3	0.040403642747
C2	C3	0.81863354305
C1	C4	0.0072447271091
C2	C4	0.045022776629
C3	C4	0.87380721638
C1	N5	0.0027259949107
C2	N5	0.016406668747
C3	N5	0.059833439897

C4	N5	1.9122992251
C1	H6	0.0069787065493
C2	H6	0.028017334033
C3	H6	0.80066760129
C4	H6	0.040664513103
N5	H6	0.01516382636
C1	H7	0.0069494477795
C2	H7	0.027964250439
C3	H7	0.80065478675
C4	H7	0.04066458087
N5	H7	0.015163985904
H6	H7	0.028443988815
C1	H8	0.032748685459
C2	H8	0.81326256159
C3	H8	0.034698525224
C4	H8	0.0080066482234
N5	H8	0.0029801788322
H6	H8	0.0082434861871
H7	H8	0.0028177925923
C1	H9	0.032742701833
C2	H9	0.81329465944
C3	H9	0.034726180063
C4	H9	0.0080069298156
N5	H9	0.0029799237606
H6	H9	0.0028182263172
H7	H9	0.0082435794168
H8	H9	0.031506647571
C1	C1	0.82690687896
C2	C1	0.03330233217
C3	C1	0.006806385609
C4	C1	0.00065285485483
N5	C1	0.0003864301211
H6	C1	0.006738288765
H7	C1	0.00050544297929
H8	C1	0.008929373361
H9	C1	0.0030256696896
C1	H11	0.82945854899
C2	H11	0.033309234401
C3	H11	0.0081020067963
C4	H11	0.0016179145807
N5	H11	0.00066636272233
H6	H11	0.00071449892524
H7	H11	0.0007145997286
H8	H11	0.0030882158368
H9	H11	0.0030886025993
C1	H11	0.032981066895
C1	H12	0.82680368526
C2	H12	0.033248947599

C3	H12	0.0068074150301
C4	H12	0.00065286849221
N5	H12	0.00038643681478
H6	H12	0.00050537804609
H7	H12	0.0067386921143
H8	H12	0.0030259401872
H9	H12	0.0089293503257
C1	H12	0.033739031128
H11	H12	0.032980783035



## ISOCYANOFORMONITRILE



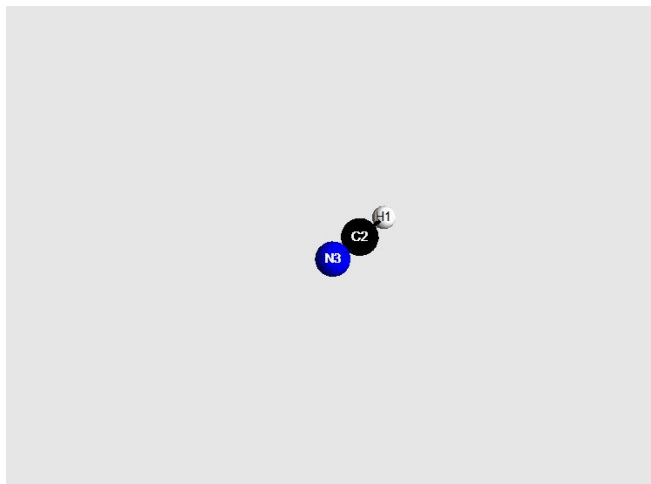
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.9028504478
N1	N3	0.25586826295
C2	N3	2.1683113209
N1	C4	1.6067681119
C2	C4	0.02081611995
N3	C4	0.078051562627

### CCSD

Atom A	Atom B	Delocalization index
N1	C2	0.89948056873
N1	N3	0.14477345883
C2	N3	1.8751800565
N1	C4	1.4651362854
C2	C4	0.021266899577
N3	C4	0.058513973176

## HYDROGEN CYANIDE



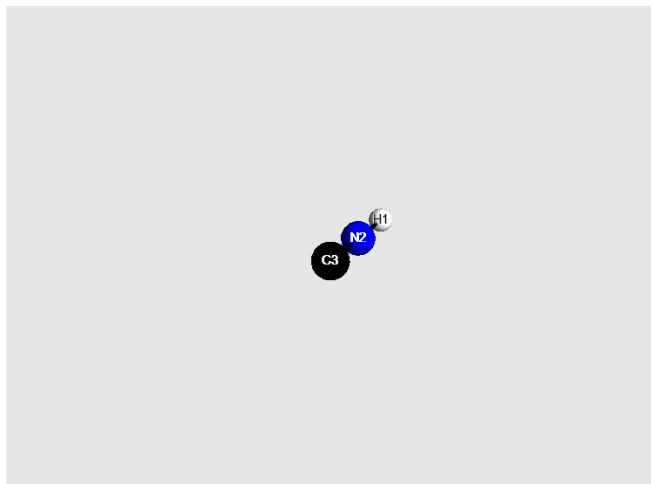
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	C2	0.92783056184
H1	N3	0.086058081245
C2	N3	2.3399366081

### CCSD

Atom A	Atom B	Delocalization index
H1	C2	0.81631676577
H1	N3	0.061912316594
C2	N3	1.9767703517

## HYDROGEN ISOCYANIDE



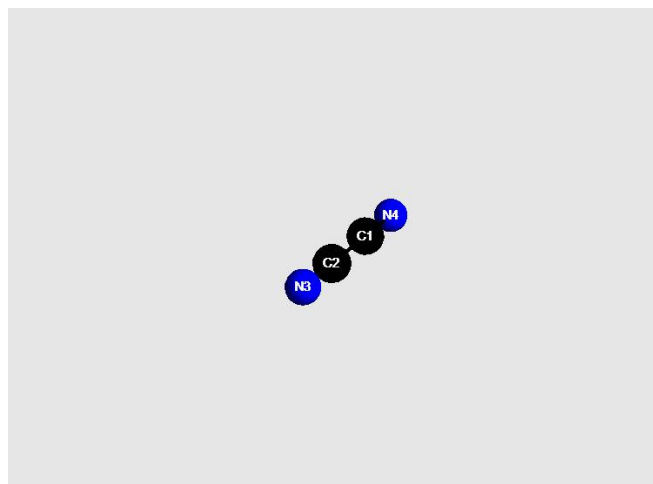
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	N2	0.66808196818
H1	C3	0.023095231881
N2	C3	1.7665072039

### CCSD

Atom A	Atom B	Delocalization index
H1	N2	0.64803803697
H1	C3	0.024518995719
N2	C3	1.5865128593

## CYANOGEN



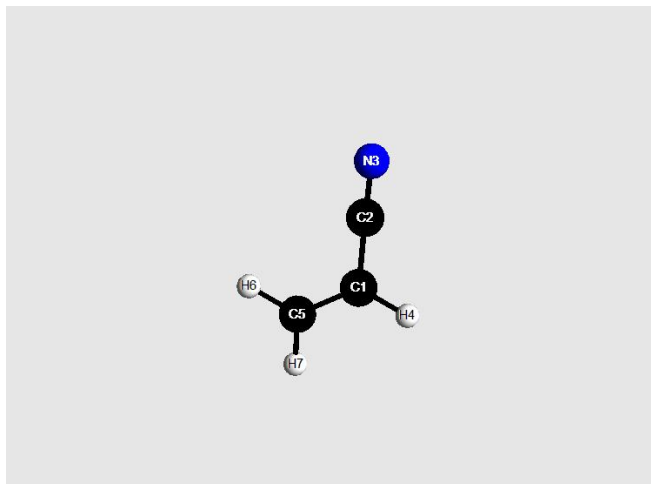
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.0787899887
C1	N3	0.10711710448
C2	N3	2.2991904698
C1	N4	2.2992236278
C2	N4	0.10711553806
N3	N4	0.11326018577

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.98264152313
C1	N3	0.068220574968
C2	N3	1.9134418957
C1	N4	1.9134422275
C2	N4	0.068220570478
N3	N4	0.073610972285

## ACRYLONITRILE



### HARTREE-FOCK

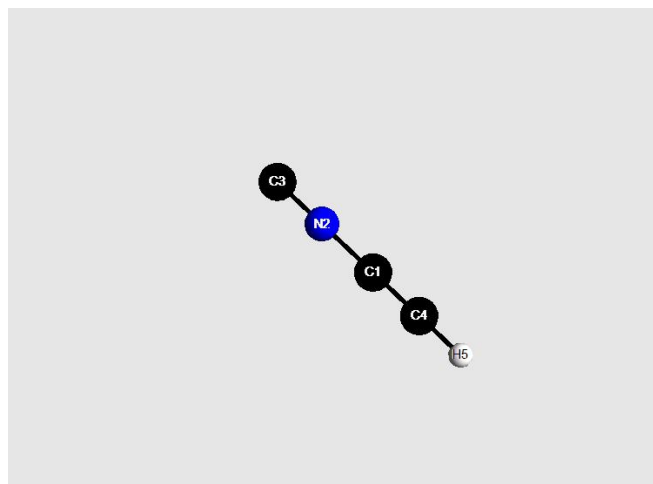
Atom A	Atom B	Delocalization index
C1	C2	1.049023161
C1	N3	0.090337327051
C2	N3	2.230303882
C1	H4	0.95499918726
C2	H4	0.043802700712
N3	H4	0.017070656086
C1	C5	1.8009197961
C2	C5	0.090140816162
N3	C5	0.068520544655
H4	C5	0.055298412615
C1	H6	0.061821974481
C2	H6	0.010734604906
N3	H6	0.005596046089
H4	H6	0.010979386776
C5	H6	0.96879340079
C1	H7	0.063301928658
C2	H7	0.010880363333
N3	H7	0.0052889010693
H4	H7	0.0068466840898
C5	H7	0.97362332395
H6	H7	0.032775714399

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.93750596716
C1	N3	0.063125450386
C2	N3	1.9019410862
C1	H4	0.82464699748
C2	H4	0.03321791377
N3	H4	0.012447449257

C1	C5	1.4345970862
C2	C5	0.061628188592
N3	C5	0.045337142812
H4	C5	0.040649681213
C1	H6	0.044356656211
C2	H6	0.010072823249
N3	H6	0.0041054391306
H4	H6	0.0091142534338
C5	H6	0.83807987721
C1	H7	0.04555603854
C2	H7	0.0082163927156
N3	H7	0.0039748925824
H4	H7	0.0054906866125
C5	H7	0.84272389923
H6	H7	0.02626403299

## ISOCYANOETHYNE



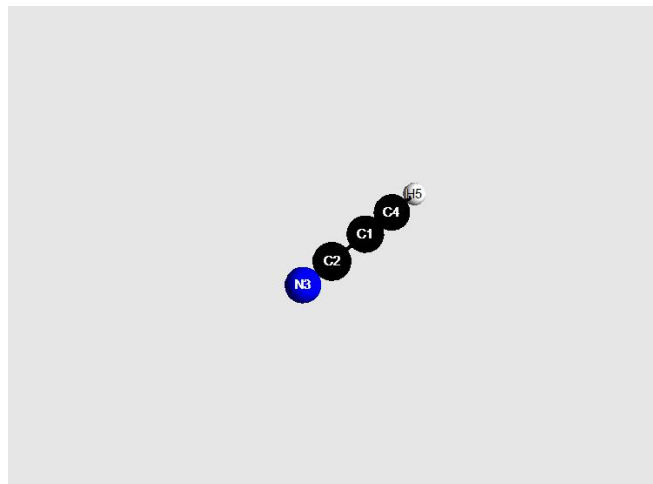
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	N2	1.0068724175
C1	C3	0.044102192918
N2	C3	1.656188671
C1	C4	2.4709190996
N2	C4	0.17571455759
C3	C4	0.071666163624
C1	H5	0.078778768441
N2	H5	0.0062453840843
C3	H5	0.0024731538892
C4	H5	0.95206615066

### CCSD

Atom A	Atom B	Delocalization index
C1	N2	0.95052416585
C1	C3	0.03440432018
N2	C3	1.4954862943
C1	C4	2.0222100646
N2	C4	0.10814952329
C3	C4	0.05745613246
C1	H5	0.05127148657
N2	H5	0.0042967023523
C3	H5	0.0021957414765
C4	H5	0.83643302075

## PROPIOLONITRILE



### HARTREE-FOCK

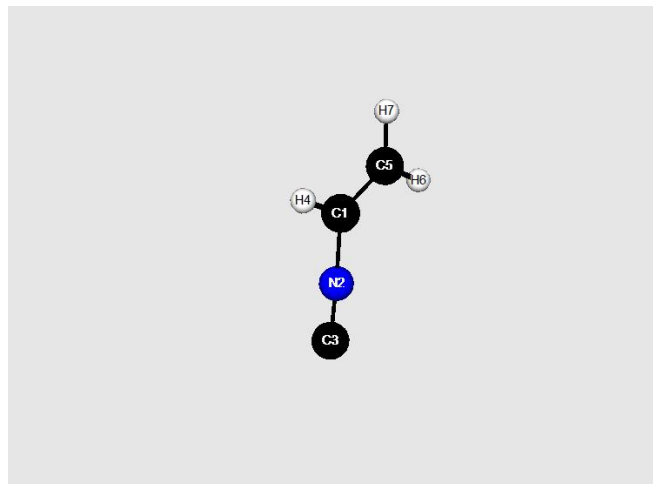
Atom A	Atom B	Delocalization index
C1	C2	1.125097298
C1	N3	0.10151021379
C2	N3	2.2439011777
C1	C4	1.7305309211
C2	C4	0.074244749423
N3	C4	0.10594028053
C1	H5	0.052905337789
C2	H5	0.002412593904
N3	H5	0.0036761712976
C4	H5	0.94520681146

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.0330082699
C1	N3	0.07329984058
C2	N3	1.8888033469
C1	C4	2.0903575111
C2	C4	0.05550529046
N3	C4	0.076553965232
C1	H5	0.047371233487
C2	H5	0.002115590802
N3	H5	0.0027875567628
C4	H5	0.83677479163



## ISOCYANOETHENE



### HARTREE-FOCK

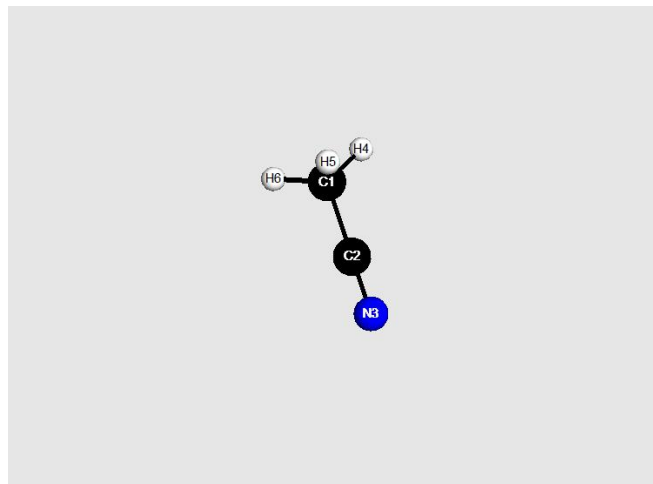
Atom A	Atom B	Delocalization index
C1	N2	0.87129755266
C1	C3	0.032299157304
N2	C3	1.7384044225
C1	H4	0.9340275096
N2	H4	0.069210700233
C3	H4	0.011110734417
C1	C5	1.7579763749
N2	C5	0.14827341458
C3	C5	0.044223508941
H4	C5	0.053064190179
C1	H6	0.064032390559
N2	H6	0.01631747142
C3	H6	0.0024077129184
H4	H6	0.010269089447
C5	H6	0.96872303389
C1	H7	0.068174453669
N2	H7	0.014508236851
C3	H7	0.0031406042752
H4	H7	0.0059895087826
C5	H7	0.97501656602
H6	H7	0.032479541331

### CCSD

Atom A	Atom B	Delocalization index
C1	N2	0.8285453281
C1	C3	0.028361566425
N2	C3	1.5568663104
C1	H4	0.80925397013
N2	H4	0.049953682643
C3	H4	0.0091811785224

C1	C5	1.4118448598
N2	C5	0.098445105213
C3	C5	0.032787328882
H4	C5	0.039205139893
C1	H6	0.04401674149
N2	H6	0.013827767942
C3	H6	0.0021490190073
H4	H6	0.0084982316412
C5	H6	0.83783555176
C1	H7	0.04755134651
N2	H7	0.010474274257
C3	H7	0.0027681558678
H4	H7	0.004766783827
C5	H7	0.84395406617
H6	H7	0.025500112362

## ACETONITRILE



### HARTREE-FOCK

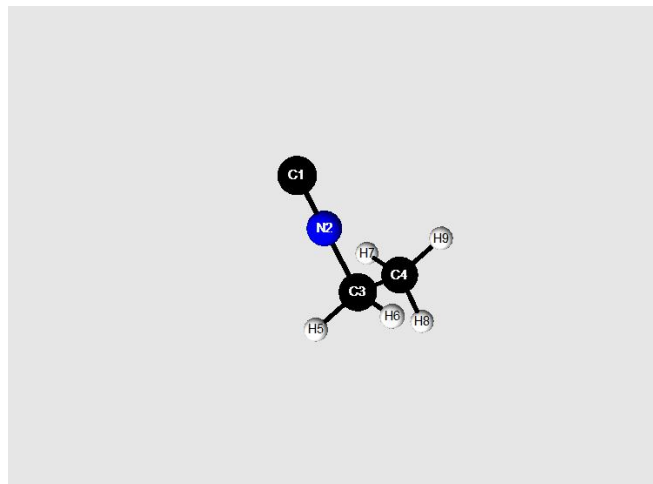
Atom A	Atom B	Delocalization index
C1	C2	1.0053076296
C1	N3	0.086190688275
C2	N3	2.2397401565
C1	H4	0.9469505444
C2	H4	0.052330853826
N3	H4	0.021871622622
C1	H5	0.94689769506
C2	H5	0.052325922045
N3	H5	0.021875619767
H4	H5	0.034527095931
C1	H6	0.94686616371
C2	H6	0.052323024954
N3	H6	0.021875079991
H4	H6	0.034525966627
H5	H6	0.034524733539

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.89462147638
C1	N3	0.062599373511
C2	N3	1.9203267794
C1	H4	0.8170389731
C2	H4	0.0391831576
N3	H4	0.015810520731
C1	H5	0.81702329158
C2	H5	0.039194163839
N3	H5	0.015812625521
H4	H5	0.027979604757
C1	H6	0.81703254078
C2	H6	0.039206534825

N3	H6	0.0158130978
H4	H6	0.027970364184
H5	H6	0.027970408853

## ISOCYANOETHANE



### HARTREE-FOCK

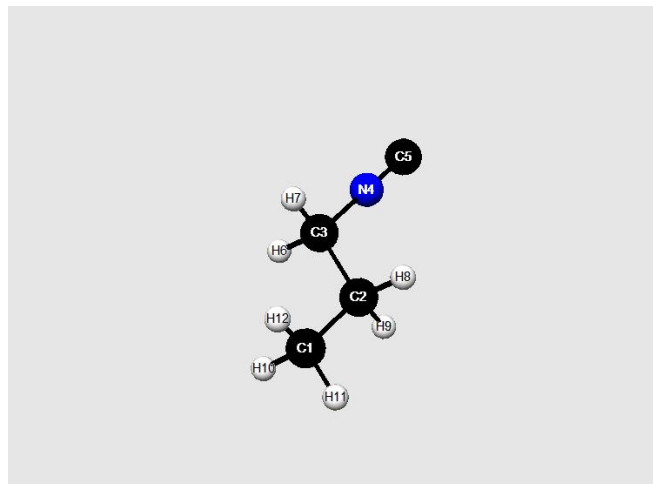
Atom A	Atom B	Delocalization index
C1	N2	1.7845938794
C1	C3	0.030738165019
N2	C3	0.8032373197
C1	C4	0.012837097628
N2	C4	0.085264702575
C3	C4	0.95321014716
C1	H5	0.012968670959
N2	H5	0.076903220902
C3	H5	0.91660063214
C4	H5	0.035943344502
C1	H6	0.012968541534
N2	H6	0.076902395428
C3	H6	0.91657563195
C4	H6	0.035934720345
H5	H6	0.03458460251
C1	H7	0.001139757169
N2	H7	0.011341291877
C3	H7	0.041991438246
C4	H7	0.96080869474
H5	H7	0.0033909346709
H6	H7	0.010340685819
C1	H8	0.0022700310977
N2	H8	0.012815302066
C3	H8	0.043873750563
C4	H8	0.96491695031
H5	H8	0.0033037047561
H6	H8	0.0033038564115
H7	H8	0.040263477942
C1	H9	0.0011398225198
N2	H9	0.011341462749

C3	H9	0.041937711345
C4	H9	0.96082753521
H5	H9	0.010340651175
H6	H9	0.0033907663245
H7	H9	0.04020135291
H8	H9	0.040263087873

### CCSD

Atom A	Atom B	Delocalization index
C1	N2	1.5899608144
C1	C3	0.028271834423
N2	C3	0.76364126391
C1	C4	0.010947359407
N2	C4	0.067272518719
C3	C4	0.82493561296
C1	H5	0.010641002695
N2	H5	0.0560852018
C3	H5	0.79108777257
C4	H5	0.02957084204
C1	H6	0.010641057379
N2	H6	0.05608483787
C3	H6	0.79091241908
C4	H6	0.029571271896
H5	H6	0.027546388686
C1	H7	0.001236840625
N2	H7	0.010424090211
C3	H7	0.033082300541
C4	H7	0.82574181655
H5	H7	0.002940308384
H6	H7	0.0083512349208
C1	H8	0.0022006485302
N2	H8	0.0096404352513
C3	H8	0.034663355281
C4	H8	0.82938691256
H5	H8	0.0029203570345
H6	H8	0.0029206285019
H7	H8	0.031239176038
C1	H9	0.0012369708127
N2	H9	0.010424800756
C3	H9	0.033065504056
C4	H9	0.82572184355
H5	H9	0.0083512456348
H6	H9	0.0029396390687
H7	H9	0.031300155268
H8	H9	0.031239054453

## ISOCYANOPROPANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	0.98135880094
C1	C3	0.046599759863
C2	C3	0.93681870529
C1	N4	0.011601601142
C2	N4	0.082263744119
C3	N4	0.80280190956
C1	C5	0.002104662056
C2	C5	0.012483490032
C3	C5	0.030676416227
N4	C5	1.7852751486
C1	H6	0.0070595091901
C2	H6	0.034041833089
C3	H6	0.91300725337
N4	H6	0.076715060419
C5	H6	0.012897913188
C1	H7	0.0070681420533
C2	H7	0.033999558758
C3	H7	0.91301691794
N4	H7	0.076713418177
C5	H7	0.012891817932
H6	H7	0.034766627102
C1	H8	0.040280992291
C2	H8	0.94731126037
C3	H8	0.042362249037
N4	H8	0.012718834253
C5	H8	0.0012682308654
H6	H8	0.0099991176288
H7	H8	0.0033916519632
C1	H9	0.040274899555
C2	H9	0.94717786005

C3	H9	0.042366693123
N4	H9	0.012711720215
C5	H9	0.0012683512532
H6	H9	0.0033934717662
H7	H9	0.009999542299
H8	H9	0.040119774241
C1	C1	0.96343969355
C2	C1	0.042094688355
C3	C1	0.0069739484251
N4	C1	0.0010447458812
C5	C1	0.00022423032721
H6	C1	0.0058791848236
H7	C1	0.00047430165405
H8	C1	0.011134365738
H9	C1	0.0034510093081
C1	H11	0.96473571652
C2	H11	0.042187559461
C3	H11	0.010226889487
N4	H11	0.0021851608452
C5	H11	0.00046987014698
H6	H11	0.00082306123572
H7	H11	0.00082377233726
H8	H11	0.0036073227222
H9	H11	0.0036078071917
C1	H11	0.042681796753
C1	H12	0.96342183554
C2	H12	0.042050807376
C3	H12	0.0069673984689
N4	H12	0.0010445261872
C5	H12	0.00022421277551
H6	H12	0.0004739486659
H7	H12	0.0058818893309
H8	H12	0.0034512372354
H9	H12	0.011133931798
C1	H12	0.043606980036
H11	H12	0.042681910537

#### CCSD

Atom A	Atom B	Delocalization index
C1	C2	0.84386279264
C1	C3	0.040236482625
C2	C3	0.80962180598
C1	N4	0.0086013275011
C2	N4	0.064398210108
C3	N4	0.76418724643
C1	C5	0.0019818988041
C2	C5	0.01060970953
C3	C5	0.028163033454

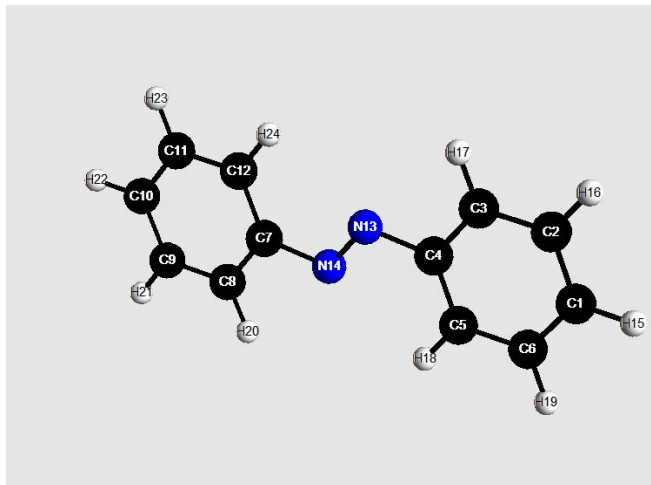


N4	C5	1.590112182
C1	H6	0.0068601731587
C2	H6	0.0278958442
C3	H6	0.78659595818
N4	H6	0.055717612507
C5	H6	0.010555314211
C1	H7	0.0068057533613
C2	H7	0.027863864346
C3	H7	0.78657488902
N4	H7	0.055716247992
C5	H7	0.010552628861
H6	H7	0.02755686485
C1	H8	0.032353736661
C2	H8	0.81201170717
C3	H8	0.033613511797
N4	H8	0.011626473588
C5	H8	0.0013480979669
H6	H8	0.008128317581
H7	H8	0.0029462990355
C1	H9	0.032351318412
C2	H9	0.81205950995
C3	H9	0.033526987194
N4	H9	0.011628787951
C5	H9	0.0013491576072
H6	H9	0.0029454998086
H7	H9	0.0081282577634
H8	H9	0.031144578637
C1	C1	0.82736681583
C2	C1	0.033231207318
C3	C1	0.0065402566721
N4	C1	0.00089571087484
C5	C1	0.00024738673411
H6	C1	0.006716941959
H7	C1	0.00050071642643
H8	C1	0.0088742011704
H9	C1	0.0029896911231
C1	H11	0.82926710037
C2	H11	0.033435732801
C3	H11	0.0079280944784
N4	H11	0.0017559118297
C5	H11	0.00048624017127
H6	H11	0.00074270630959
H7	H11	0.00074258840105
H8	H11	0.0030872074022
H9	H11	0.0030874477276
C1	H11	0.03301911046
C1	H12	0.82718680381
C2	H12	0.033188345719

C3	H12	0.0065291640538
N4	H12	0.00089565782403
C5	H12	0.00024735004987
H6	H12	0.00050072303425
H7	H12	0.0067151203227
H8	H12	0.0029897955853
H9	H12	0.0088740870261
C1	H12	0.033721204181
H11	H12	0.033019218348

# DIAZOCOMPOUNDS

## DIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.4026723114
C1	C3	0.074767622104
C2	C3	1.3752109881
C1	C4	0.087918267817
C2	C4	0.070979722739
C3	C4	1.3382416406
C1	C5	0.073532098951
C2	C5	0.096179268354
C3	C5	0.066659713258
C4	C5	1.3071103469
C1	C6	1.3626379267
C2	C6	0.07355157456
C3	C6	0.093091023927
C4	C6	0.073614574045
C5	C6	1.4150536967
C1	C7	0.00075342628573
C2	C7	0.000419605177
C3	C7	0.002153180809
C4	C7	0.013334274289
C5	C7	0.0020806190813
C6	C7	0.00024461046821
C1	C8	0.0016075220786
C2	C8	0.00027165687759
C3	C8	0.0024369659334
C4	C8	0.0021531866769
C5	C8	0.0019625193912
C6	C8	0.0002510771603
C7	C8	1.3382419298

C1	C9	0.00017284129381
C2	C9	3.7386922346e-05
C3	C9	0.0002716566913
C4	C9	0.00041960518332
C5	C9	0.00020285863002
C6	C9	3.4658600117e-05
C7	C9	0.070979742425
C8	C9	1.3752109041
C1	C1	0.0012202946468
C2	C1	0.00017284063937
C3	C1	0.0016075225148
C4	C1	0.00075342701713
C5	C1	0.0013123334335
C6	C1	0.00016587961115
C7	C1	0.087918201138
C8	C1	0.074767593516
C9	C1	1.4026725633
C1	C11	0.0001658790372
C2	C11	3.4659098576e-05
C3	C11	0.00025107655367
C4	C11	0.00024460871864
C5	C11	0.00025448223432
C6	C11	3.3049818975e-05
C7	C11	0.073614556959
C8	C11	0.093091041369
C9	C11	0.073551513303
C1	C11	1.3626377608
C1	C12	0.0013123323774
C2	C12	0.00020285851869
C3	C12	0.0019625167775
C4	C12	0.00208064078
C5	C12	0.0019638377417
C6	C12	0.00025448387004
C7	C12	1.3071109229
C8	C12	0.066659672946
C9	C12	0.09617931982
C1	C12	0.073532051367
C11	C12	1.4150537706
C1	N13	0.0096023015227
C2	N13	0.0097992150406
C3	N13	0.090278500087
C4	N13	0.97051417145
C5	N13	0.069264027788
C6	N13	0.012007788486
C7	N13	0.068801075299
C8	N13	0.033253996367
C9	N13	0.0039641057374
C1	N13	0.015106037418

C11	N13	0.0050560682668
C12	N13	0.049963058597
C1	N14	0.015106080664
C2	N14	0.0039641726588
C3	N14	0.033254017497
C4	N14	0.068801811343
C5	N14	0.049963035729
C6	N14	0.0050561444686
C7	N14	0.97051452838
C8	N14	0.090278871699
C9	N14	0.0097992171403
C1	N14	0.0096023119254
C11	N14	0.012007799147
C12	N14	0.069263999874
N13	N14	1.9900230963
C1	H15	0.97605658429
C2	H15	0.049315076806
C3	H15	0.0086356924179
C4	H15	0.0055695742308
C5	H15	0.0083830690058
C6	H15	0.04782553832
C7	H15	6.0256954922e-05
C8	H15	0.00011177175184
C9	H15	1.2081712755e-05
C1	H15	8.5859957984e-05
C11	H15	1.2218397282e-05
C12	H15	9.296621491e-05
N13	H15	0.00061435464134
N14	H15	0.001052305144
C1	H16	0.049410004752
C2	H16	0.97618685628
C3	H16	0.04883888804
C4	H16	0.008305067271
C5	H16	0.006007755291
C6	H16	0.0086357186336
C7	H16	7.5372855534e-05
C8	H16	1.7948675897e-05
C9	H16	3.8840897396e-06
C1	H16	6.4174298844e-06
C11	H16	2.6992493499e-06
C12	H16	9.3575535649e-06
N13	H16	0.0011614019998
N14	H16	0.00034906368357
H15	H16	0.0056107554473
C1	H17	0.0081555672812
C2	H17	0.045360630531
C3	H17	0.96505721702
C4	H17	0.044733923226

C5	H17	0.0075570436791
C6	H17	0.0056523765361
C7	H17	0.00025040452157
C8	H17	0.00010262436887
C9	H17	1.4851201023e-05
C1	H17	6.4941149776e-05
C11	H17	1.7880403482e-05
C12	H17	0.0001356281353
N13	H17	0.021364683148
N14	H17	0.0025145171089
H15	H17	0.0012921038166
H16	H17	0.005469796598
C1	H18	0.0077556626046
C2	H18	0.00528615898
C3	H18	0.0073455303706
C4	H18	0.041375421106
C5	H18	0.95407302279
C6	H18	0.045282334574
C7	H18	0.0012372835177
C8	H18	0.00019389141092
C9	H18	1.8071492955e-05
C1	H18	5.6337684065e-05
C11	H18	6.7654224498e-05
C12	H18	0.00036682532844
N13	H18	0.0069847883991
N14	H18	0.033443638255
H15	H18	0.001179048695
H16	H18	0.00033716033961
H17	H18	0.0014980478433
C1	H19	0.048155192054
C2	H19	0.0084636322212
C3	H19	0.0058188917817
C4	H19	0.0084708123556
C5	H19	0.050433930452
C6	H19	0.9754377672
C7	H19	4.6938989385e-05
C8	H19	1.296839551e-05
C9	H19	2.4173265095e-06
C1	H19	7.5521480539e-06
C11	H19	2.2322668158e-06
C12	H19	2.4216747465e-05
N13	H19	0.0018875779053
N14	H19	0.00028446983625
H15	H19	0.0054845369426
H16	H19	0.0014080596491
H17	H19	0.00035876850724
H18	H19	0.0056453489727
C1	C2	6.4939858613e-05

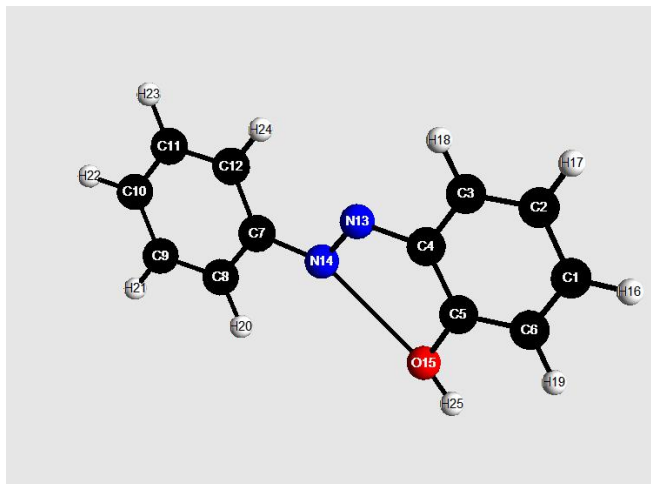
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C4	C2	0.00025040263589
C5	C2	0.0001356256673
C6	C2	1.7880166969e-05
C7	C2	0.044733638983
C8	C2	0.96505520681
C9	C2	0.045360418077
C1	C2	0.0081555253354
C11	C2	0.0056522977309
C12	C2	0.0075570353485
N13	C2	0.0025144955745
N14	C2	0.021364608859
H15	C2	4.6192095552e-06
H16	C2	1.7401377775e-06
H17	C2	1.2885646761e-05
H18	C2	0.00014908742051
H19	C2	1.9631526407e-06
C1	H21	6.4179601808e-06
C2	H21	3.8838179097e-06
C3	H21	1.7948959658e-05
C4	H21	7.537292998e-05
C5	H21	9.3579179965e-06
C6	H21	2.6998419221e-06
C7	H21	0.0083050537685
C8	H21	0.048838690374
C9	H21	0.97618638877
C1	H21	0.049409831134
C11	H21	0.0086356960332
C12	H21	0.0060077001162
N13	H21	0.00034905832433
N14	H21	0.0011614003832
H15	H21	4.7481121871e-07
H16	H21	8.9136170113e-07
H17	H21	1.7403360279e-06
H18	H21	1.7081297755e-06
H19	H21	3.0768767833e-07
C2	H21	0.0054697785167
C1	H22	8.5860183397e-05
C2	H22	1.2081699366e-05
C3	H22	0.00011177143249
C4	H22	6.0256455392e-05
C5	H22	9.2965400384e-05
C6	H22	1.2218706328e-05
C7	H22	0.0055695594917
C8	H22	0.0086356966388
C9	H22	0.049315070498
C1	H22	0.97605614655

C11	H22	0.047825488997
C12	H22	0.0083830778953
N13	H22	0.0010522991983
N14	H22	0.00061435319125
H15	H22	5.7971994697e-06
H16	H22	4.7466537308e-07
H17	H22	4.6195182426e-06
H18	H22	3.8684037044e-06
H19	H22	6.58619744e-07
C2	H22	0.0012920981133
H21	H22	0.0056107444564
C1	H23	7.5520301241e-06
C2	H23	2.4169313538e-06
C3	H23	1.2968394902e-05
C4	H23	4.6938668992e-05
C5	H23	2.4215799329e-05
C6	H23	2.2320798607e-06
C7	H23	0.008470810174
C8	H23	0.0058188830321
C9	H23	0.0084636242003
C1	H23	0.048155153452
C11	H23	0.97543749719
C12	H23	0.05043390654
N13	H23	0.00028446593184
N14	H23	0.0018875769683
H15	H23	6.5858161671e-07
H16	H23	3.075997037e-07
H17	H23	1.9631847124e-06
H18	H23	2.188743735e-05
H19	H23	5.3560017776e-07
C2	H23	0.000358763619
H21	H23	0.0014080577064
H22	H23	0.0054845318731
C1	H24	5.6337539843e-05
C2	H24	1.807142693e-05
C3	H24	0.00019388849061
C4	H24	0.0012372722084
C5	H24	0.00036682236898
C6	H24	6.7653205198e-05
C7	H24	0.041375548453
C8	H24	0.0073455243657
C9	H24	0.0052861967176
C1	H24	0.0077556653782
C11	H24	0.045282337745
C12	H24	0.95407576613
N13	H24	0.033443438324
N14	H24	0.0069847052834
H15	H24	3.8686024108e-06



H16	H24	1.7080897759e-06
H17	H24	0.00014908728021
H18	H24	4.1211246169e-05
H19	H24	2.188732246e-05
C2	H24	0.0014980473122
H21	H24	0.00033716004057
H22	H24	0.0011790482399
H23	H24	0.0056453517664

## O-HYDROXYDIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3809450324
C1	C3	0.079833495386
C2	C3	1.3933317781
C1	C4	0.082954631023
C2	C4	0.067140051181
C3	C4	1.3186105643
C1	C5	0.071605904072
C2	C5	0.080796888781
C3	C5	0.068366005672
C4	C5	1.2423329141
C1	C6	1.387396658
C2	C6	0.072775139306
C3	C6	0.092297320158
C4	C6	0.063053568107
C5	C6	1.311184229
C1	C7	0.00072798991032
C2	C7	0.0003820953843
C3	C7	0.0020590822787
C4	C7	0.013624846133
C5	C7	0.0014221409107
C6	C7	0.00028085177913
C1	C8	0.0015750672102
C2	C8	0.00029247227769
C3	C8	0.0023014201933
C4	C8	0.0024158666288
C5	C8	0.0019697143074
C6	C8	0.0002206670862
C7	C8	1.3378798677
C1	C9	0.0001686500053
C2	C9	4.1746196606e-05

C3	C9	0.00025698279851
C4	C9	0.00046584324589
C5	C9	0.0002060328749
C6	C9	2.9553955599e-05
C7	C9	0.071123591603
C8	C9	1.3762245201
C1	C1	0.0012001150387
C2	C1	0.00018813306678
C3	C1	0.0015139228184
C4	C1	0.00089437840826
C5	C1	0.0013415528092
C6	C1	0.00015380687404
C7	C1	0.088201064079
C8	C1	0.074514303772
C9	C1	1.4020203016
C1	C11	0.00016503185799
C2	C11	3.4067314795e-05
C3	C11	0.00024261223205
C4	C11	0.00025765919619
C5	C11	0.00022045218375
C6	C11	2.5634710202e-05
C7	C11	0.073360652011
C8	C11	0.093230071828
C9	C11	0.073599598497
C1	C11	1.3638986929
C1	C12	0.0012976523695
C2	C12	0.00022161162457
C3	C12	0.0018872692482
C4	C12	0.0022316275509
C5	C12	0.0018250959785
C6	C12	0.00021570757082
C7	C12	1.3088824088
C8	C12	0.067048199953
C9	C12	0.096220029186
C1	C12	0.073352300991
C11	C12	1.4141829272
C1	N13	0.0088933707344
C2	N13	0.01009643526
C3	N13	0.092388590379
C4	N13	0.99957256052
C5	N13	0.066701093999
C6	N13	0.0091534332633
C7	N13	0.07006194212
C8	N13	0.032465593184
C9	N13	0.0039153474006
C1	N13	0.014633924485
C11	N13	0.0050630014094
C12	N13	0.050102262071

C1	N14	0.014726934809
C2	N14	0.0038773744809
C3	N14	0.032224492348
C4	N14	0.068174886856
C5	N14	0.027749462817
C6	N14	0.0025557090517
C7	N14	0.9757907751
C8	N14	0.088935912834
C9	N14	0.0096785090758
C1	N14	0.0092985780298
C11	N14	0.011894733192
C12	N14	0.068362785591
N13	N14	1.9781152952
C1	O15	0.015144351225
C2	O15	0.019241294776
C3	O15	0.011010295152
C4	O15	0.092533621553
C5	O15	0.84423390121
C6	O15	0.12095572759
C7	O15	0.0021508647606
C8	O15	0.00073380681542
C9	O15	7.1797860426e-05
C1	O15	0.00032185376142
C11	O15	0.00015691290309
C12	O15	0.00089234734375
N13	O15	0.013185859607
N14	O15	0.070180909086
C1	H16	0.97338094175
C2	H16	0.046828118138
C3	H16	0.0087070146722
C4	H16	0.005233274032
C5	H16	0.0081753553428
C6	H16	0.049091618087
C7	H16	5.6079065188e-05
C8	H16	0.00011105898182
C9	H16	1.1944701423e-05
C1	H16	8.5950222541e-05
C11	H16	1.202718069e-05
C12	H16	9.1410326964e-05
N13	H16	0.00057076557916
N14	H16	0.00095500666465
O15	H16	0.0016366167296
C1	H17	0.049255074862
C2	H17	0.9785480772
C3	H17	0.050005493889
C4	H17	0.0085037292769
C5	H17	0.0052674529058
C6	H17	0.0088966217723

C7	H17	7.3071583502e-05
C8	H17	2.0383703997e-05
C9	H17	4.1754996014e-06
C1	H17	8.8941965205e-06
C11	H17	3.2818218554e-06
C12	H17	1.2705462142e-05
N13	H17	0.0010902858379
N14	H17	0.00036554738992
O15	H17	0.0014902211964
H16	H17	0.0053860907525
C1	H18	0.0083966214968
C2	H18	0.044846610764
C3	H18	0.95973104019
C4	H18	0.043606767509
C5	H18	0.0072047326537
C6	H18	0.0055260324413
C7	H18	0.00030566219742
C8	H18	9.7087519363e-05
C9	H18	1.5974342315e-05
C1	H18	5.7439567701e-05
C11	H18	2.279840037e-05
C12	H18	0.00016182498379
N13	H18	0.026047059291
N14	H18	0.0027643141907
O15	H18	0.0015341118433
H16	H18	0.0014187456673
H17	H18	0.0055498752157
C1	H19	0.048339257057
C2	H19	0.0086524033648
C3	H19	0.0061435096866
C4	H19	0.0068452179636
C5	H19	0.050213735948
C6	H19	0.97180267267
C7	H19	4.3689757687e-05
C8	H19	1.1527840093e-05
C9	H19	2.1873274648e-06
C1	H19	5.0850519915e-06
C11	H19	2.4415416659e-06
C12	H19	2.3070026721e-05
N13	H19	0.002039703454
N14	H19	0.00028902082917
O15	H19	0.01926248444
H16	H19	0.005991767968
H17	H19	0.0013911667987
H18	H19	0.0003509325253
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C2	C2	1.5895205522e-05
C3	C2	9.646834733e-05

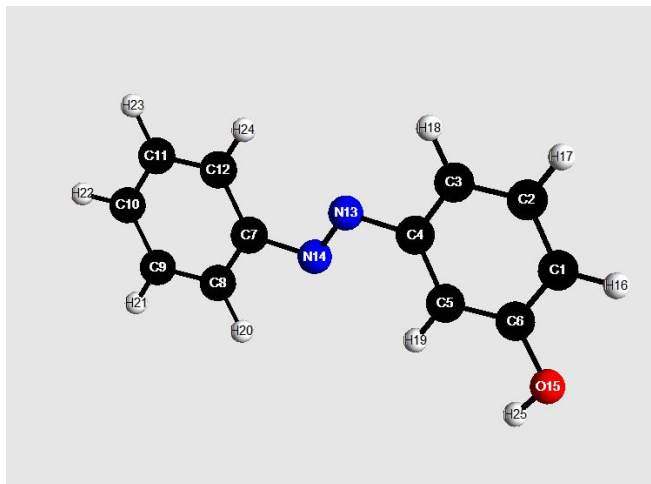
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C8	C2	0.96409095824
C9	C2	0.045179978673
C1	C2	0.0081197339461
C11	C2	0.0055786491604
C12	C2	0.0074920326199
N13	C2	0.0023655833526
N14	C2	0.020600414834
O15	C2	0.00053212974028
H16	C2	4.8081926021e-06
H17	C2	1.4392101892e-06
H18	C2	1.3827485162e-05
H19	C2	2.5908134077e-06
C1	H21	6.246808568e-06
C2	H21	3.7937199012e-06
C3	H21	1.6429628479e-05
C4	H21	7.8796696378e-05
C5	H21	9.9910224102e-06
C6	H21	2.3964130971e-06
C7	H21	0.0083304231799
C8	H21	0.048958654531
C9	H21	0.97672223219
C1	H21	0.049620219342
C11	H21	0.0086743102671
C12	H21	0.0060568452067
N13	H21	0.0003466111897
N14	H21	0.0011496334653
O15	H21	7.4360671644e-06
H16	H21	4.5471950967e-07
H17	H21	8.0191841094e-07
H18	H21	2.2918271072e-06
H19	H21	4.4661582889e-07
C2	H21	0.0054571245674
C1	H22	8.465078406e-05
C2	H22	1.3766607853e-05
C3	H22	0.00010604538478
C4	H22	7.2499244548e-05
C5	H22	9.5865189557e-05
C6	H22	1.0937429691e-05
C7	H22	0.0056466098999
C8	H22	0.0086564318409
C9	H22	0.049488877229
C1	H22	0.97672493555
C11	H22	0.048103226783
C12	H22	0.0084232703061

N13	H22	0.0010380677662
N14	H22	0.0006042538587
O15	H22	2.3736938864e-05
H16	H22	5.8117828457e-06
H17	H22	6.8719279011e-07
H18	H22	4.3337668126e-06
H19	H22	5.1055796465e-07
C2	H22	0.0012916934889
H21	H22	0.0056345035079
C1	H23	7.3431428899e-06
C2	H23	2.3230526291e-06
C3	H23	1.3145421673e-05
C4	H23	4.8323730557e-05
C5	H23	1.182316765e-05
C6	H23	1.956498265e-06
C7	H23	0.0084768427127
C8	H23	0.0058895063591
C9	H23	0.0085123640976
C1	H23	0.048434025518
C11	H23	0.97604173806
C12	H23	0.050593389998
N13	H23	0.00029445297501
N14	H23	0.0019030934083
O15	H23	3.8701327722e-05
H16	H23	5.4176103235e-07
H17	H23	3.4697535832e-07
H18	H23	2.2963410305e-06
H19	H23	3.797313951e-07
C2	H23	0.00035624025132
H21	H23	0.0014205197292
H22	H23	0.0055169409936
C1	H24	5.7375941103e-05
C2	H24	2.1937878206e-05
C3	H24	0.0002410306759
C4	H24	0.0012702172714
C5	H24	0.00038179862331
C6	H24	6.3297913029e-05
C7	H24	0.041463039129
C8	H24	0.0073824522846
C9	H24	0.0053439680105
C1	H24	0.0077806063913
C11	H24	0.045593510895
C12	H24	0.95481366201
N13	H24	0.034021522635
N14	H24	0.0070291834176
O15	H24	7.4448864896e-05
H16	H24	4.6603161468e-06
H17	H24	2.6070776774e-06

H18	H24	0.00024597473998
H19	H24	2.0106148167e-05
C2	H24	0.0014916330972
H21	H24	0.00034387567641
H22	H24	0.0011877875435
H23	H24	0.005680292387
C1	H25	0.00048415940065
C2	H25	0.00028298407061
C3	H25	0.00073517751037
C4	H25	0.0053741054459
C5	H25	0.010421042965
C6	H25	0.0062472364674
C7	H25	8.9791898601e-05
C8	H25	1.0899908527e-05
C9	H25	6.9932284155e-07
C1	H25	2.9290326123e-06
C11	H25	4.9583902552e-06
C12	H25	2.9947057092e-05
N13	H25	0.00025992649344
N14	H25	0.0017528206979
O15	H25	0.57631370331
H16	H25	6.416107164e-05
H17	H25	4.985929364e-05
H18	H25	0.0002162060089
H19	H25	0.0053413559391
C2	H25	4.4386978372e-06
H21	H25	1.5861534141e-07
H22	H25	2.3147527087e-07
H23	H25	2.2691084247e-06
H24	H25	6.4025273765e-06



## M-HYDROXYDIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.4241249427
C1	C3	0.07115273393
C2	C3	1.3558859278
C1	C4	0.086023157115
C2	C4	0.074253128404
C3	C4	1.3514478483
C1	C5	0.063763340407
C2	C5	0.092453871612
C3	C5	0.066931301808
C4	C5	1.2988636641
C1	C6	1.2737262285
C2	C6	0.075832132692
C3	C6	0.080553251353
C4	C6	0.073263551068
C5	C6	1.3540352867
C1	C7	0.00075239572058
C2	C7	0.00043581158575
C3	C7	0.0021965217263
C4	C7	0.01337693024
C5	C7	0.0020587659419
C6	C7	0.00024931113386
C1	C8	0.0016300244913
C2	C8	0.00028288776495
C3	C8	0.0026136096603
C4	C8	0.0020778957793
C5	C8	0.0017676172266
C6	C8	0.00023785282777
C7	C8	1.3380393627
C1	C9	0.00017558282691
C2	C9	3.8159614066e-05

C3	C9	0.00028980918763
C4	C9	0.00041202704051
C5	C9	0.00018433275425
C6	C9	3.3258895936e-05
C7	C9	0.070883696081
C8	C9	1.3751998477
C1	C1	0.0012385177224
C2	C1	0.00018152048121
C3	C1	0.0017407256769
C4	C1	0.00070192823011
C5	C1	0.0011740191755
C6	C1	0.00015696409388
C7	C1	0.0878444024
C8	C1	0.074892304994
C9	C1	1.4026594367
C1	C11	0.00016737980464
C2	C11	3.6262260416e-05
C3	C11	0.00026894649461
C4	C11	0.00023603659413
C5	C11	0.00023653998657
C6	C11	3.1984653768e-05
C7	C11	0.073681070785
C8	C11	0.093047240605
C9	C11	0.073482414941
C1	C11	1.3624241652
C1	C12	0.0013249713012
C2	C12	0.00020903023312
C3	C12	0.0021032917516
C4	C12	0.0020243791574
C5	C12	0.001823806812
C6	C12	0.00024650251224
C7	C12	1.306635199
C8	C12	0.066590487101
C9	C12	0.096107074873
C1	C12	0.073665203944
C11	C12	1.4151467919
C1	N13	0.0098125291785
C2	N13	0.010031895349
C3	N13	0.090937759556
C4	N13	0.96927847651
C5	N13	0.068652277603
C6	N13	0.011820770687
C7	N13	0.068620818455
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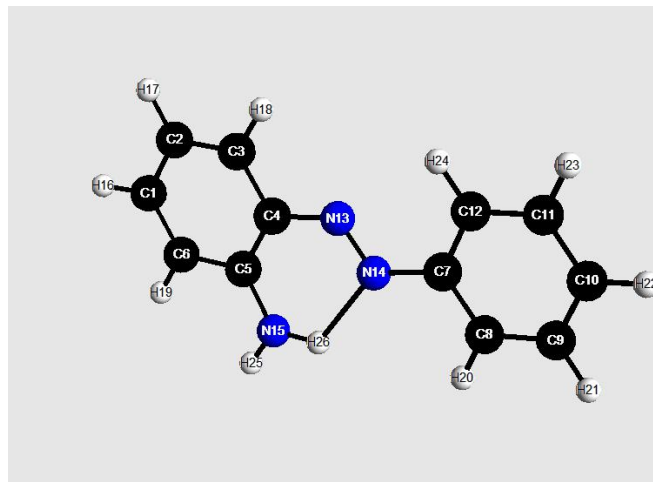
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H22	H25	9.9191411275e-08
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## O-AMINODIAZOBENZENE



### HARTREE-FOCK

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H17	H19	0.0013958256882
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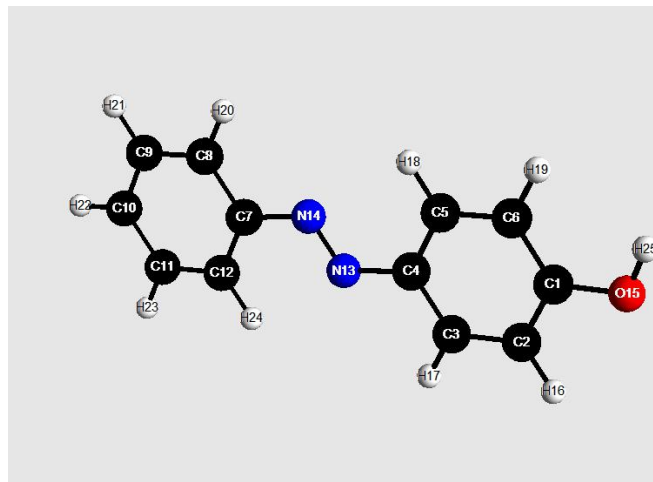
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C12	C2	0.0076250338284
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N15	C2	0.00054496273167
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C1	H25	0.00058495844654
C2	H25	0.00076283033231
C3	H25	0.0010248318994
C4	H25	0.0072111611291
C5	H25	0.01830507626
C6	H25	0.0071283012184
C7	H25	0.00018774937595
C8	H25	3.9111470235e-05
C9	H25	3.4495453011e-06
C1	H25	1.8509925365e-05
C11	H25	1.2052044811e-05
C12	H25	7.1218232941e-05
N13	H25	0.00059888128612
N14	H25	0.003253320262
N15	H25	0.82338810714
H16	H25	5.8547869453e-05
H17	H25	8.0854919661e-05
H18	H25	0.00027919850322
H19	H25	0.005640891614
C2	H25	1.1152644624e-05
H21	H25	1.6543904517e-07
H22	H25	1.3445000226e-06
H23	H25	4.4897250906e-06
H24	H25	1.1526424618e-05
C1	H26	0.0010664903902
C2	H26	0.00063815267176
C3	H26	0.00019714697173
C4	H26	0.003045909598
C5	H26	0.014273109795
C6	H26	0.0059024499446
C7	H26	0.0015760247741
C8	H26	0.00056097999546
C9	H26	5.626139405e-05
C1	H26	4.2322442956e-05
C11	H26	8.3818174583e-05
C12	H26	0.00049254578424
N13	H26	0.0034270091766
N14	H26	0.053530541861
N15	H26	0.71024641537
H16	H26	0.00019170916803
H17	H26	5.3183422812e-05
H18	H26	3.8563174095e-05

H19	H26	0.00054847183805
C2	H26	0.0007654126781
H21	H26	5.8128301104e-06
H22	H26	5.7728112989e-06
H23	H26	2.7435986034e-05
H24	H26	4.4335518909e-05
H25	H26	0.012474564701

## P-HYDROXYDIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3105993824
C1	C3	0.078311286535
C2	C3	1.3938444767
C1	C4	0.07549468505
C2	C4	0.068314686378
C3	C4	1.3219411398
C1	C5	0.073371794874
C2	C5	0.091832488414
C3	C5	0.069093336584
C4	C5	1.3075328601
C1	C6	1.2950000795
C2	C6	0.063137433298
C3	C6	0.088000456094
C4	C6	0.071237247759
C5	C6	1.4136605931
C1	C7	0.00065245775398
C2	C7	0.00041521690863
C3	C7	0.0020995276166
C4	C7	0.01323328745
C5	C7	0.0021296702673
C6	C7	0.00026749904651
C1	C8	0.0014385922771
C2	C8	0.00029918828709
C3	C8	0.002359885168
C4	C8	0.0023932226289
C5	C8	0.0020821381499
C6	C8	0.00033574943773
C7	C8	1.3383292452
C1	C9	0.00015625074087
C2	C9	4.2392395508e-05



C3	C9	0.00026464829249
C4	C9	0.00045120757586
C5	C9	0.00021536820165
C6	C9	4.4623941574e-05
C7	C9	0.07096614615
C8	C9	1.3755279202
C1	C1	0.0010900561294
C2	C1	0.00019319683864
C3	C1	0.001549376012
C4	C1	0.00091675574682
C5	C1	0.0013942431901
C6	C1	0.00022630729439
C7	C1	0.088064622158
C8	C1	0.074461613533
C9	C1	1.4022654254
C1	C11	0.00014797589366
C2	C11	3.6684540573e-05
C3	C11	0.00024321784783
C4	C11	0.00026717692336
C5	C11	0.00026681643414
C6	C11	4.1510431438e-05
C7	C11	0.073591647837
C8	C11	0.093179565326
C9	C11	0.073672140499
C1	C11	1.3633661426
C1	C12	0.0011759443203
C2	C12	0.00023108732212
C3	C12	0.0019079204889
C4	C12	0.0022413050354
C5	C12	0.0020575064322
C6	C12	0.00031254272473
C7	C12	1.3079236205
C8	C12	0.066746265585
C9	C12	0.096154644314
C1	C12	0.073261075007
C11	C12	1.4142863548
C1	N13	0.0089885113054
C2	N13	0.0099293942974
C3	N13	0.090229003503
C4	N13	0.97756204851
C5	N13	0.072056306951
C6	N13	0.012974853384
C7	N13	0.068519208018
C8	N13	0.032774679415
C9	N13	0.0039288969969
C1	N13	0.01479309414
C11	N13	0.0050166462025
C12	N13	0.049661448497

C1	N14	0.013763396415
C2	N14	0.0042895198646
C3	N14	0.032736827304
C4	N14	0.071157057726
C5	N14	0.050959830787
C6	N14	0.0058093977215
C7	N14	0.97237575844
C8	N14	0.08919185611
C9	N14	0.0097619343005
C1	N14	0.0092450063119
C11	N14	0.011944479673
C12	N14	0.068754281922
N13	N14	1.9845517557
C1	O15	0.83262675358
C2	O15	0.11044309839
C3	O15	0.013811335595
C4	O15	0.016965414202
C5	O15	0.014597022427
C6	O15	0.11305610846
C7	O15	0.00017411586581
C8	O15	0.00040958681244
C9	O15	4.572648314e-05
C1	O15	0.00031448630118
C11	O15	4.2479627397e-05
C12	O15	0.00033480038879
N13	O15	0.002448627871
N14	O15	0.0037888970262
C1	H16	0.046821253051
C2	H16	0.96832181042
C3	H16	0.046312474989
C4	H16	0.0080315243731
C5	H16	0.0054880619618
C6	H16	0.0067722443669
C7	H16	7.1843604684e-05
C8	H16	1.8479203421e-05
C9	H16	3.7857263954e-06
C1	H16	7.1566806986e-06
C11	H16	2.6350514566e-06
C12	H16	1.061881354e-05
N13	H16	0.0010976760013
N14	H16	0.00035244656631
O15	H16	0.01526261052
C1	H17	0.0080886734761
C2	H17	0.045728419176
C3	H17	0.96249225596
C4	H17	0.042968307219
C5	H17	0.0076017779167
C6	H17	0.0052972295141

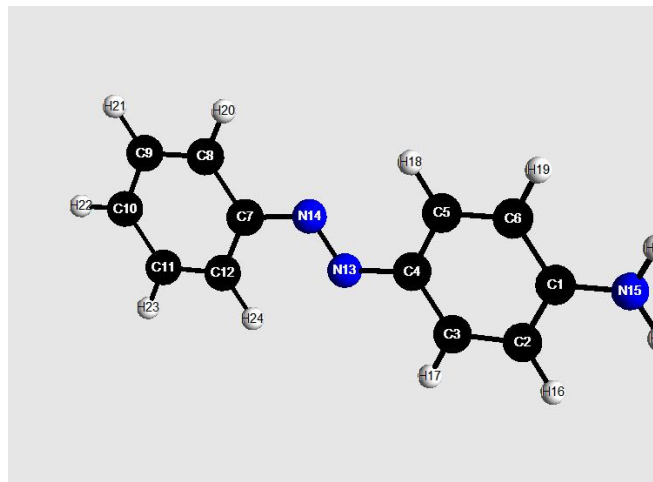
C7	H17	0.0002469981501
C8	H17	9.7371785743e-05
C9	H17	1.4273116299e-05
C1	H17	6.1577757103e-05
C11	H17	1.7333146585e-05
C12	H17	0.00013160109586
N13	H17	0.020743742786
N14	H17	0.0024514832486
O15	H17	0.0013471854677
H16	H17	0.0056017826161
C1	H18	0.007549935323
C2	H18	0.004969944107
C3	H18	0.0073926561894
C4	H18	0.039734469652
C5	H18	0.95153910059
C6	H18	0.045428654451
C7	H18	0.0012415935438
C8	H18	0.00018976907116
C9	H18	1.7815663079e-05
C1	H18	5.7369335478e-05
C11	H18	6.7572395161e-05
C12	H18	0.00036668450464
N13	H18	0.0070287215453
N14	H18	0.032797817526
O15	H18	0.0015065159887
H16	H18	0.00027757853412
H17	H18	0.0015649106518
C1	H19	0.048752628908
C2	H19	0.0069900883568
C3	H19	0.0058310029243
C4	H19	0.0083808442462
C5	H19	0.049423035216
C6	H19	0.97311216871
C7	H19	4.8685805307e-05
C8	H19	1.7210361863e-05
C9	H19	2.7238676972e-06
C1	H19	1.0524819057e-05
C11	H19	2.5772088754e-06
C12	H19	2.6801593643e-05
N13	H19	0.0018850437119
N14	H19	0.0003401669939
O15	H19	0.015899684793
H16	H19	0.001695893791
H17	H19	0.00033046031394
H18	H19	0.0058740801328
C1	C2	5.9255158802e-05
C2	C2	1.6855190659e-05
C3	C2	0.00010054022374

C4	C2	0.00025930542152
C5	C2	0.00013759529178
C6	C2	2.0325402242e-05
C7	C2	0.044828325207
C8	C2	0.96536618468
C9	C2	0.045582255013
C1	C2	0.0081781193147
C11	C2	0.005685686352
C12	C2	0.0075647763779
N13	C2	0.002525287245
N14	C2	0.021487159883
O15	C2	1.6824005303e-05
H16	C2	1.6628617755e-06
H17	C2	1.2700495272e-05
H18	C2	0.00014124779584
H19	C2	2.1659214546e-06
C1	H21	5.8844098389e-06
C2	H21	3.9676002836e-06
C3	H21	1.7566940774e-05
C4	H21	7.5102144637e-05
C5	H21	9.7707243228e-06
C6	H21	2.9550056143e-06
C7	H21	0.0083162749165
C8	H21	0.048890422437
C9	H21	0.97632930296
C1	H21	0.049468764289
C11	H21	0.0086570499905
C12	H21	0.0060386006443
N13	H21	0.0003485493434
N14	H21	0.0011588879304
O15	H21	1.6398517326e-06
H16	H21	8.2834809052e-07
H17	H21	1.6961367148e-06
H18	H21	1.6573659271e-06
H19	H21	3.143712544e-07
C2	H21	0.0055004751997
C1	H22	7.837765108e-05
C2	H22	1.4911599683e-05
C3	H22	0.00010883773947
C4	H22	7.682681064e-05
C5	H22	9.9666869719e-05
C6	H22	1.7651888018e-05
C7	H22	0.0056076527743
C8	H22	0.0086489003141
C9	H22	0.049425220774
C1	H22	0.97637982547
C11	H22	0.047988340535
C12	H22	0.008401099656

N13	H22	0.0010396386427
N14	H22	0.00060437171677
O15	H22	2.3836800484e-05
H16	H22	5.8620061982e-07
H17	H22	4.4196351072e-06
H18	H22	3.9288807741e-06
H19	H22	9.1839183805e-07
C2	H22	0.0012966943318
H21	H22	0.0056201316435
C1	H23	6.5719476864e-06
C2	H23	2.301472086e-06
C3	H23	1.2623716983e-05
C4	H23	4.6762587147e-05
C5	H23	2.4707090444e-05
C6	H23	2.5254305299e-06
C7	H23	0.008473008337
C8	H23	0.0058476998797
C9	H23	0.0084847647985
C1	H23	0.048225745656
C11	H23	0.97551869733
C12	H23	0.050449208838
N13	H23	0.00028302460548
N14	H23	0.001886072468
O15	H23	1.8414044957e-06
H16	H23	2.8909941406e-07
H17	H23	1.9523024056e-06
H18	H23	2.2007310436e-05
H19	H23	5.7230522814e-07
C2	H23	0.00036223693608
H21	H23	0.0014151623309
H22	H23	0.005496133347
C1	H24	5.3266391497e-05
C2	H24	1.8078371171e-05
C3	H24	0.00019350522866
C4	H24	0.0012255551622
C5	H24	0.00037733322406
C6	H24	7.2265504543e-05
C7	H24	0.041440088577
C8	H24	0.0073411501426
C9	H24	0.0053067958035
C1	H24	0.0077636808951
C11	H24	0.045388490378
C12	H24	0.95445652178
N13	H24	0.033599194646
N14	H24	0.0069956927046
O15	H24	1.6450128235e-05
H16	H24	1.7892082158e-06
H17	H24	0.00014610906577

H18	H24	4.1421046714e-05
H19	H24	2.1143029756e-05
C2	H24	0.0015056805986
H21	H24	0.00033998529685
H22	H24	0.0011822589821
H23	H24	0.005666043434
C1	H25	0.010149263267
C2	H25	0.0055493336127
C3	H25	0.00094679941821
C4	H25	0.00023463511676
C5	H25	0.00040208831281
C6	H25	0.0049624553646
C7	H25	3.094198098e-06
C8	H25	3.3217713287e-06
C9	H25	5.0459116691e-07
C1	H25	2.3667079147e-06
C11	H25	3.9061082807e-07
C12	H25	3.0047704426e-06
N13	H25	6.7198084369e-05
N14	H25	3.233859708e-05
O15	H25	0.5749740131
H16	H25	0.00034563463044
H17	H25	0.00018769971145
H18	H25	4.7372315467e-05
H19	H25	0.0039398779756
C2	H25	2.0148933949e-07
H21	H25	3.1101479676e-08
H22	H25	1.8455404264e-07
H23	H25	4.3305498244e-08
H24	H25	6.3625439012e-07

## P-AMINODIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.3005477235
C1	C3	0.074649149859
C2	C3	1.3967021947
C1	C4	0.070600694298
C2	C4	0.068909374396
C3	C4	1.3223428727
C1	C5	0.073110143744
C2	C5	0.08578863783
C3	C5	0.068929607492
C4	C5	1.2854906638
C1	C6	1.2621025415
C2	C6	0.063052354202
C3	C6	0.083838469083
C4	C6	0.070372519996
C5	C6	1.4418740247
C1	C7	0.00064137382739
C2	C7	0.00046144507109
C3	C7	0.0021328238803
C4	C7	0.013210012029
C5	C7	0.0020698889718
C6	C7	0.00029451511022
C1	C8	0.0014518247674
C2	C8	0.00040481930944
C3	C8	0.0024818934174
C4	C8	0.0026231189087
C5	C8	0.0019871175554
C6	C8	0.00039705362713
C7	C8	1.3381228852
C1	C9	0.00016039410094
C2	C9	5.7489653545e-05

C3	C9	0.00028010785606
C4	C9	0.0004918722756
C5	C9	0.00020727728417
C6	C9	5.5644473011e-05
C7	C9	0.071003735094
C8	C9	1.376438169
C1	C1	0.0011087244339
C2	C1	0.00027625365659
C3	C1	0.0016390776685
C4	C1	0.0010886806546
C5	C1	0.0013276925028
C6	C1	0.00027379863386
C7	C1	0.088190524146
C8	C1	0.074144219055
C9	C1	1.4017312383
C1	C11	0.00015132134478
C2	C11	4.8847478084e-05
C3	C11	0.00025611210202
C4	C11	0.0002945568693
C5	C11	0.00025884633484
C6	C11	4.8473037603e-05
C7	C11	0.073543562884
C8	C11	0.093287518765
C9	C11	0.073857836198
C1	C11	1.3643152249
C1	C12	0.0011952512387
C2	C12	0.00032526757758
C3	C12	0.002019685777
C4	C12	0.0024126296694
C5	C12	0.0019890184391
C6	C12	0.00035937715474
C7	C12	1.3087274442
C8	C12	0.067017359885
C9	C12	0.09615686834
C1	C12	0.072970040402
C11	C12	1.4138041237
C1	N13	0.0092492019782
C2	N13	0.010679725034
C3	N13	0.093052568849
C4	N13	0.98203377241
C5	N13	0.072802678397
C6	N13	0.013921210879
C7	N13	0.068703454186
C8	N13	0.032218530544
C9	N13	0.0038938992262
C1	N13	0.014426959092
C11	N13	0.004972335736
C12	N13	0.049409235903



C1	N14	0.013927512493
C2	N14	0.0052904524275
C3	N14	0.034313057092
C4	N14	0.072968329512
C5	N14	0.049688366633
C6	N14	0.0064368513308
C7	N14	0.97716423677
C8	N14	0.088094694282
C9	N14	0.0097235396728
C1	N14	0.0088760778608
C11	N14	0.011868066114
C12	N14	0.068114147304
N13	N14	1.976061283
C1	N15	0.98507111933
C2	N15	0.11083688273
C3	N15	0.015648612735
C4	N15	0.021323600316
C5	N15	0.015241414401
C6	N15	0.10546139363
C7	N15	0.00025794755506
C8	N15	0.00063256060657
C9	N15	7.458080728e-05
C1	N15	0.00049580164723
C11	N15	6.7602909323e-05
C12	N15	0.00052160860131
N13	N15	0.0038333300073
N14	N15	0.0057087485064
C1	H16	0.048674914495
C2	H16	0.97624778446
C3	H16	0.049654352346
C4	H16	0.0084152507945
C5	H16	0.0056044555289
C6	H16	0.007343894192
C7	H16	7.5525826822e-05
C8	H16	2.5635051486e-05
C9	H16	4.7739208755e-06
C1	H16	1.2365895727e-05
C11	H16	3.3988636961e-06
C12	H16	1.6665201182e-05
N13	H16	0.0011816583377
N14	H16	0.00042744586869
N15	H16	0.01444017998
C1	H17	0.0080719645299
C2	H17	0.046245379414
C3	H17	0.96307375286
C4	H17	0.043098009976
C5	H17	0.007743894345
C6	H17	0.0052201381824

C7	H17	0.00025087516711
C8	H17	0.00010325122221
C9	H17	1.5029865055e-05
C1	H17	6.6744078664e-05
C11	H17	1.8445076851e-05
C12	H17	0.00013949790905
N13	H17	0.020871281599
N14	H17	0.002526202828
N15	H17	0.0013819890648
H16	H17	0.0059319038055
C1	H18	0.0077374103922
C2	H18	0.0046531959974
C3	H18	0.007412489751
C4	H18	0.039087895964
C5	H18	0.95233452893
C6	H18	0.046619035855
C7	H18	0.0012455540552
C8	H18	0.0001789962619
C9	H18	1.6721276655e-05
C1	H18	5.1552587577e-05
C11	H18	6.6256679287e-05
C12	H18	0.00036093505642
N13	H18	0.00694133621
N14	H18	0.032468916809
N15	H18	0.0013012355191
H16	H18	0.00029471721026
H17	H18	0.0015675357395
C1	H19	0.047022594594
C2	H19	0.0071202459617
C3	H19	0.0054701051272
C4	H19	0.0084904369423
C5	H19	0.051324591501
C6	H19	0.97448391385
C7	H19	4.9085086682e-05
C8	H19	2.0089817927e-05
C9	H19	3.2113663216e-06
C1	H19	1.2757233635e-05
C11	H19	2.9669143747e-06
C12	H19	2.9183976647e-05
N13	H19	0.0019322913782
N14	H19	0.00037260161328
N15	H19	0.014482865128
H16	H19	0.0017462321121
H17	H19	0.00032662173678
H18	H19	0.0060822393326
C1	C2	6.0501959707e-05
C2	C2	2.2082276102e-05
C3	C2	0.00010653783129

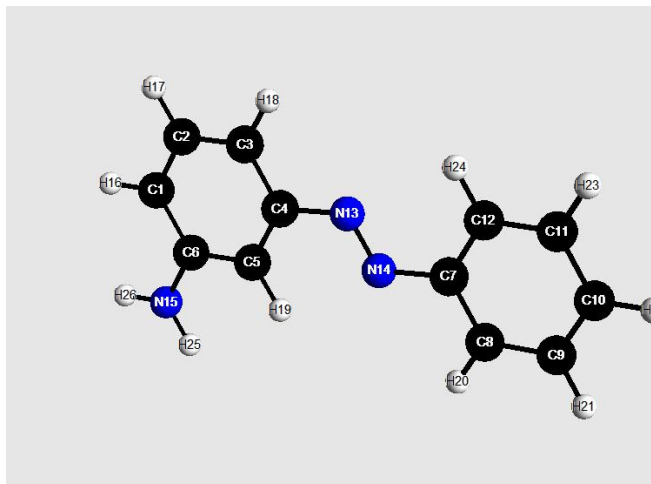
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C8	C2	0.96569481935
C9	C2	0.045804842097
C1	C2	0.008197572039
C11	C2	0.0057016465989
C12	C2	0.0075651374868
N13	C2	0.0025333954084
N14	C2	0.021583164104
N15	C2	2.6754240688e-05
H16	C2	1.9751933322e-06
H17	C2	1.3127866294e-05
H18	C2	0.00013648452502
H19	C2	2.3255799858e-06
C1	H21	5.7888139611e-06
C2	H21	4.422480127e-06
C3	H21	1.7949949426e-05
C4	H21	7.5098495451e-05
C5	H21	9.287560621e-06
C6	H21	3.2785922751e-06
C7	H21	0.0083326706759
C8	H21	0.049027777975
C9	H21	0.97673899428
C1	H21	0.049605087282
C11	H21	0.0086961761488
C12	H21	0.0060861475617
N13	H21	0.000348802941
N14	H21	0.0011550429762
N15	H21	2.5560830244e-06
H16	H21	8.7788938454e-07
H17	H21	1.7499499549e-06
H18	H21	1.5676012651e-06
H19	H21	3.2854109653e-07
C2	H21	0.0055317724231
C1	H22	8.1632509886e-05
C2	H22	2.2478656638e-05
C3	H22	0.00011728035699
C4	H22	9.4705964813e-05
C5	H22	9.6869774571e-05
C6	H22	2.2274007886e-05
C7	H22	0.0056720083314
C8	H22	0.0086786528116
C9	H22	0.049625813147
C1	H22	0.97708258345
C11	H22	0.048232185877
C12	H22	0.0084381507289

N13	H22	0.0010291701669
N14	H22	0.00059740781626
N15	H22	3.8630412514e-05
H16	H22	1.0390580237e-06
H17	H22	4.8717934065e-06
H18	H22	3.6082526273e-06
H19	H22	1.1314552427e-06
C2	H22	0.0013026742987
H21	H22	0.0056391474659
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C2	H23	2.6476015164e-06
C3	H23	1.2797310291e-05
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C5	H23	2.4226531933e-05
C6	H23	2.7257300403e-06
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C8	H23	0.0059059647888
C9	H23	0.0085330527313
C1	H23	0.048438767313
C11	H23	0.9760170541
C12	H23	0.050578311544
N13	H23	0.00028267169032
N14	H23	0.0018910145092
N15	H23	2.6108699901e-06
H16	H23	3.0302472563e-07
H17	H23	1.9657248529e-06
H18	H23	2.1971787045e-05
H19	H23	5.7924153854e-07
C2	H23	0.00036633302658
H21	H23	0.0014276361542
H22	H23	0.0055217537585
C1	H24	5.8045464922e-05
C2	H24	2.2807776056e-05
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C9	H24	0.0053339086398
C1	H24	0.0077765704708
C11	H24	0.045594569428
C12	H24	0.95490807158
N13	H24	0.033908737013
N14	H24	0.0069997002674
N15	H24	2.8346231034e-05
H16	H24	2.1317207074e-06
H17	H24	0.00015127642066

H18	H24	4.1191764199e-05
H19	H24	2.2010390104e-05
C2	H24	0.0015104975439
H21	H24	0.00034398892705
H22	H24	0.001188381317
H23	H24	0.0056943575789
C1	H25	0.017596443726
C2	H25	0.0075001093357
C3	H25	0.001328002778
C4	H25	0.00067724036518
C5	H25	0.00047882375052
C6	H25	0.0057483370343
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C9	H25	2.1773155092e-06
C1	H25	1.3390835211e-05
C11	H25	1.8889060734e-06
C12	H25	1.4510514258e-05
N13	H25	0.00013750629601
N14	H25	0.00015212689218
N15	H25	0.81915596794
H16	H25	0.00054283220665
H17	H25	0.00023715930958
H18	H25	4.0511745152e-05
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C2	H25	7.6106079956e-07
H21	H25	7.8970225186e-08
H22	H25	1.0245557885e-06
H23	H25	8.5768733353e-08
H24	H25	1.183781471e-06
C1	H26	0.017557894027
C2	H26	0.0057121033477
C3	H26	0.00047832219169
C4	H26	0.00065662596759
C5	H26	0.0013226615086
C6	H26	0.007408443249
C7	H26	8.2549396058e-06
C8	H26	1.7498562769e-05
C9	H26	2.0591828763e-06
C1	H26	1.3351590304e-05
C11	H26	1.9928465243e-06
C12	H26	1.4671208419e-05
N13	H26	0.00011669627763
N14	H26	0.00016353308305
N15	H26	0.81943372797
H16	H26	0.0041196485823
H17	H26	3.7879097442e-05
H18	H26	0.00022554676097

H19	H26	0.00054786701467
C2	H26	7.8268592428e-07
H21	H26	9.0673753751e-08
H22	H26	1.0202026663e-06
H23	H26	9.5496756873e-08
H24	H26	7.8152835685e-07
H25	H26	0.016221369929

## M-AMINODIAZOBENZENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
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C1	C3	0.071399649253
C2	C3	1.3628992727
C1	C4	0.083242011761
C2	C4	0.074930903067
C3	C4	1.3364299873
C1	C5	0.06553718892
C2	C5	0.090517061087
C3	C5	0.067467626247
C4	C5	1.3212508696
C1	C6	1.2718375544
C2	C6	0.072121026568
C3	C6	0.077692961192
C4	C6	0.072581327832
C5	C6	1.3227821886
C1	C7	0.00071617982265
C2	C7	0.00042982631098
C3	C7	0.0021156646119
C4	C7	0.013394469018
C5	C7	0.0020883335235
C6	C7	0.00023757815575
C1	C8	0.0015671465192
C2	C8	0.00027472864425
C3	C8	0.0024826690958
C4	C8	0.002053526419
C5	C8	0.0018524844625
C6	C8	0.00022156497067
C7	C8	1.3387326754
C1	C9	0.00016976475766
C2	C9	3.714453811e-05

C3	C9	0.000277330893
C4	C9	0.00040930717133
C5	C9	0.00019301214155
C6	C9	3.1260067963e-05
C7	C9	0.070922586108
C8	C9	1.3752151232
C1	C1	0.0011905018052
C2	C1	0.00017501371886
C3	C1	0.0016459483832
C4	C1	0.00068751970534
C5	C1	0.0012283962037
C6	C1	0.00014487141072
C7	C1	0.088007762307
C8	C1	0.074699660896
C9	C1	1.4025916398
C1	C11	0.00016182469229
C2	C11	3.5481806384e-05
C3	C11	0.00025639477395
C4	C11	0.00023328453685
C5	C11	0.00024276176541
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C8	C11	0.093133839461
C9	C11	0.073522599906
C1	C11	1.3629271609
C1	C12	0.0012796999883
C2	C12	0.00020303289978
C3	C12	0.0020023389576
C4	C12	0.0020098566365
C5	C12	0.0018891057341
C6	C12	0.00023644095707
C7	C12	1.3073318319
C8	C12	0.066744190643
C9	C12	0.09618109875
C1	C12	0.073501061263
C11	C12	1.4148226288
C1	N13	0.010009943884
C2	N13	0.010176764768
C3	N13	0.091626705511
C4	N13	0.96323018224
C5	N13	0.069491857831
C6	N13	0.011619859203
C7	N13	0.068901120651
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C9	N13	0.0039680892038
C1	N13	0.015080027013
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C1	N14	0.014892051615
C2	N14	0.0040614918709
C3	N14	0.034061241782
C4	N14	0.066948461964
C5	N14	0.049836608758
C6	N14	0.0049587066948
C7	N14	0.97175796924
C8	N14	0.089932051541
C9	N14	0.0097837424029
C1	N14	0.0095504048989
C11	N14	0.01196007809
C12	N14	0.068986207402
N13	N14	1.991824751
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C5	N15	0.11292538331
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N14	N15	0.00082083192782
C1	H16	0.975280732
C2	H16	0.050248997772
C3	H16	0.0086578895739
C4	H16	0.0054781470417
C5	H16	0.007154915653
C6	H16	0.046786381036
C7	H16	5.9635652235e-05
C8	H16	0.00011011741445
C9	H16	1.204136314e-05
C1	H16	8.5875106621e-05
C11	H16	1.2213168327e-05
C12	H16	9.1811355097e-05
N13	H16	0.00061702463679
N14	H16	0.0010874756079
N15	H16	0.014432719239
C1	H17	0.050582375987
C2	H17	0.97451815232
C3	H17	0.047571796865
C4	H17	0.0084972109638
C5	H17	0.0058279001496
C6	H17	0.008479485276

C7	H17	8.0920299888e-05
C8	H17	1.7759240898e-05
C9	H17	3.9204668836e-06
C1	H17	6.265590188e-06
C11	H17	2.6954906586e-06
C12	H17	8.807263376e-06
N13	H17	0.0012305586562
N14	H17	0.00035516537635
N15	H17	0.0014678275586
H16	H17	0.0061163171356
C1	H18	0.0084576364728
C2	H18	0.046214500576
C3	H18	0.9702037972
C4	H18	0.046026645028
C5	H18	0.0081568289691
C6	H18	0.0050997812571
C7	H18	0.00024830601148
C8	H18	0.000108127359
C9	H18	1.5436403648e-05
C1	H18	6.9373135915e-05
C11	H18	1.8814545548e-05
C12	H18	0.00014109528627
N13	H18	0.021157548781
N14	H18	0.002551107511
N15	H18	0.0019511698043
H16	H18	0.0012570923237
H17	H18	0.0054049551362
C1	H19	0.0067879071139
C2	H19	0.0052136363786
C3	H19	0.0076336466272
C4	H19	0.042032506398
C5	H19	0.95356326273
C6	H19	0.044628117999
C7	H19	0.0013036271958
C8	H19	0.00019901675254
C9	H19	1.8276931725e-05
C1	H19	5.4313380989e-05
C11	H19	6.9743034156e-05
C12	H19	0.00038052239896
N13	H19	0.0074842733522
N14	H19	0.035317553849
N15	H19	0.014061173956
H16	H19	0.0015154510781
H17	H19	0.00031732420859
H18	H19	0.0014961238726
C1	C2	6.3544819879e-05
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C3	C2	0.00010522932875

C4	C2	0.00024969550911
C5	C2	0.00013867426815
C6	C2	1.8496576798e-05
C7	C2	0.044850129613
C8	C2	0.96537405607
C9	C2	0.045483059782
C1	C2	0.0081731902928
C11	C2	0.0056787746888
C12	C2	0.0075740856276
N13	C2	0.0025393093194
N14	C2	0.021433692949
N15	C2	6.548260103e-06
H16	C2	4.6806749523e-06
H17	C2	1.8647631871e-06
H18	C2	1.3039843663e-05
H19	C2	0.00015991167222
C1	H21	6.2345086542e-06
C2	H21	4.0116561331e-06
C3	H21	1.7874520491e-05
C4	H21	7.6297649329e-05
C5	H21	8.89977851e-06
C6	H21	2.4297979138e-06
C7	H21	0.0083134814476
C8	H21	0.048914444734
C9	H21	0.97632058483
C1	H21	0.049475263128
C11	H21	0.0086485285843
C12	H21	0.0060321768451
N13	H21	0.00035100377275
N14	H21	0.0011622050218
N15	H21	6.9511200575e-07
H16	H21	4.7568780373e-07
H17	H21	9.536035159e-07
H18	H21	1.7609332498e-06
H19	H21	1.7778374361e-06
C2	H21	0.0054853283128
C1	H22	8.505650973e-05
C2	H22	1.2042997982e-05
C3	H22	0.00011655578219
C4	H22	5.4417915722e-05
C5	H22	8.6366777798e-05
C6	H22	1.0522085718e-05
C7	H22	0.0055904945358
C8	H22	0.0086449469202
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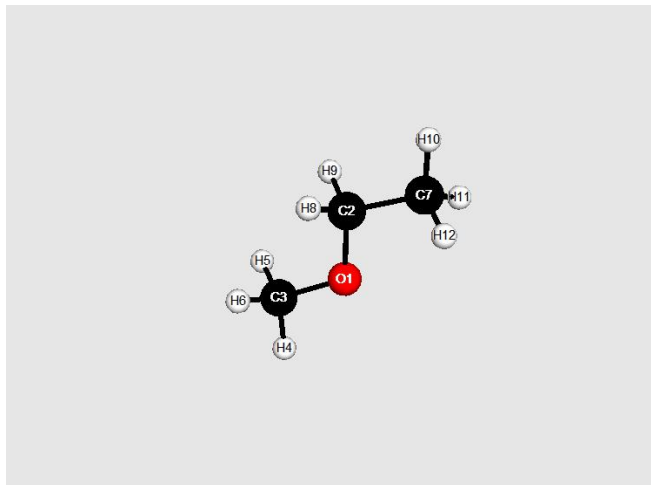
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H18	H22	5.0285014733e-06
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H21	H22	0.0056201634383
C1	H23	6.967304706e-06
C2	H23	2.4353338058e-06
C3	H23	1.2604596688e-05
C4	H23	4.670894635e-05
C5	H23	2.4245517321e-05
C6	H23	2.1560141798e-06
C7	H23	0.008472008932
C8	H23	0.0058276463925
C9	H23	0.0084709976244
C1	H23	0.048233347482
C11	H23	0.97552267758
C12	H23	0.050435849323
N13	H23	0.00028318205259
N14	H23	0.0018870263606
N15	H23	6.9223688782e-07
H16	H23	6.9416540156e-07
H17	H23	3.3739472116e-07
H18	H23	1.9076312974e-06
H19	H23	2.2786822967e-05
C2	H23	0.00036108078907
H21	H23	0.0014113366905
H22	H23	0.005491085113
C1	H24	6.0835961759e-05
C2	H24	1.9617327674e-05
C3	H24	0.00021234276929
C4	H24	0.0012430018844
C5	H24	0.00036080076687
C6	H24	6.6967599864e-05
C7	H24	0.041225819507
C8	H24	0.0073253451504
C9	H24	0.0052567905421
C1	H24	0.0077398967254
C11	H24	0.045145844157
C12	H24	0.95362993469
N13	H24	0.033596316025
N14	H24	0.0069767500384
N15	H24	2.3783756466e-05
H16	H24	3.93006441e-06
H17	H24	1.7903283517e-06

H18	H24	0.00015291501308
H19	H24	4.4356521958e-05
C2	H24	0.0014971219062
H21	H24	0.00033655686521
H22	H24	0.001178018874
H23	H24	0.0056346305756
C1	H25	0.0073835644238
C2	H25	0.0012876737101
C3	H25	0.00071204875731
C4	H25	0.00047887983477
C5	H25	0.0058971449507
C6	H25	0.01762451601
C7	H25	3.2668374301e-06
C8	H25	2.3788215544e-06
C9	H25	3.9944299604e-07
C1	H25	1.4249730074e-06
C11	H25	4.4315768329e-07
C12	H25	2.7426532702e-06
N13	H25	5.3868872035e-05
N14	H25	7.034759783e-05
N15	H25	0.82120425962
H16	H25	0.0005559799268
H17	H25	0.00024584703115
H18	H25	8.3234553525e-05
H19	H25	0.003960158007
C2	H25	2.9494984819e-07
H21	H25	4.1826954088e-08
H22	H25	1.0877551594e-07
H23	H25	7.8715729503e-08
H24	H25	4.3311977496e-07
C1	H26	0.0057094473333
C2	H26	0.0004842024428
C3	H26	0.00073018578885
C4	H26	0.0012726259098
C5	H26	0.0075358809445
C6	H26	0.017722564134
C7	H26	7.6762924654e-06
C8	H26	1.8800915945e-06
C9	H26	6.6271727156e-07
C1	H26	1.1639198059e-06
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C12	H26	3.9077109615e-06
N13	H26	0.00033399024568
N14	H26	4.1640532551e-05
N15	H26	0.82312913397
H16	H26	0.0043056344317
H17	H26	3.671122264e-05
H18	H26	7.7837941335e-05

H19	H26	0.0005519468658
C2	H26	4.816273879e-07
H21	H26	9.0094066842e-08
H22	H26	9.5645107442e-08
H23	H26	6.8268109956e-08
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# ETHERS

## ETHYL METHYL ETHER



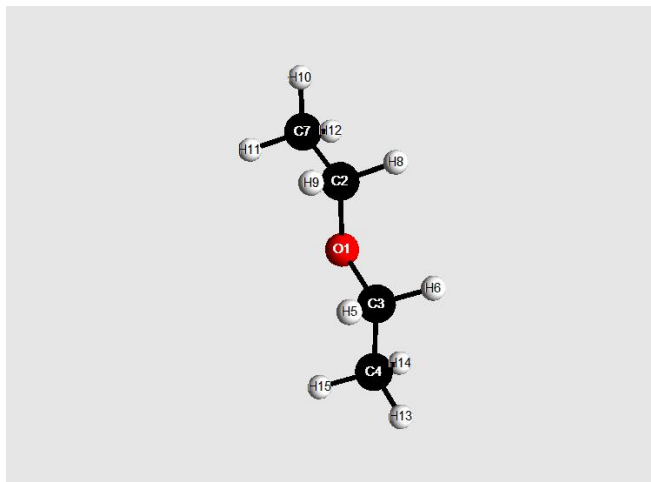
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C2	C3	0.024873231326
O1	H4	0.071669702195
C2	H4	0.0079200767485
C3	H4	0.92964948179
O1	H5	0.081665191022
C2	H5	0.0074989837479
C3	H5	0.92378413148
H4	H5	0.039601820126
O1	H6	0.081648596304
C2	H6	0.0074914409453
C3	H6	0.9237839684
H4	H6	0.039600943413
H5	H6	0.042806564221
O1	C7	0.084339429242
C2	C7	0.95258173402
C3	C7	0.0073843066151
H4	C7	0.0015728108731
H5	C7	0.00094805995948
H6	C7	0.00094783615168
O1	H8	0.081524772628
C2	H8	0.9107244304
C3	H8	0.0081945095759
H4	H8	0.00092333402954
H5	H8	0.00088534457023
H6	H8	0.010658928075
C7	H8	0.040559040494

O1	H9	0.081541736376
C2	H9	0.9108104727
C3	H9	0.0081899363732
H4	H9	0.00092325450569
H5	H9	0.010659018002
H6	H9	0.0008852490793
C7	H9	0.040564275055
H8	H9	0.041680836113
O1	O1	0.012592522218
C2	O1	0.043267520305
C3	O1	0.00157798916
H4	O1	0.00038044685525
H5	O1	9.4416553032e-05
H6	O1	9.4414801037e-05
C7	O1	0.9670045097
H8	O1	0.0036924827487
H9	O1	0.0036925008695
O1	H11	0.012003698653
C2	H11	0.04046127077
C3	H11	0.00050615386781
H4	H11	6.6787486362e-05
H5	H11	4.9071937937e-05
H6	H11	0.00041950149871
C7	H11	0.9613526428
H8	H11	0.010877646414
H9	H11	0.0039170090238
O1	H11	0.042165021617
O1	H12	0.012003909007
C2	H12	0.040463657093
C3	H12	0.00050598513866
H4	H12	6.6785555416e-05
H5	H12	0.00041951127369
H6	H12	4.906843456e-05
C7	H12	0.96135265778
H8	H12	0.0039169876776
H9	H12	0.010877625765
O1	H12	0.042165389616
H11	H12	0.041710507541



## DIETHYL ETHER



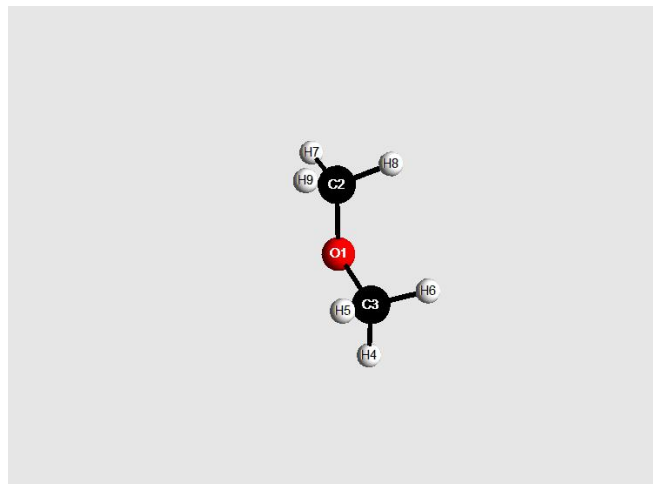
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	C2	0.78611209114
O1	C3	0.78648788313
C2	C3	0.023701281163
O1	C4	0.084600068974
C2	C4	0.0072107048748
C3	C4	0.95249616165
O1	H5	0.081344525475
C2	H5	0.007926755459
C3	H5	0.9106704088
C4	H5	0.040612629451
O1	H6	0.081272287636
C2	H6	0.0079039403494
C3	H6	0.91068300177
C4	H6	0.040639310696
H5	H6	0.041707748332
O1	C7	0.084581744168
C2	C7	0.95241639849
C3	C7	0.007208553205
C4	C7	0.001328446972
H5	C7	0.00099029426948
H6	C7	0.00099031901066
O1	H8	0.081264560054
C2	H8	0.91067564751
C3	H8	0.0079155646647
C4	H8	0.00099006889161
H5	H8	0.00090020163847
H6	H8	0.011358758796
C7	H8	0.04066197862
O1	H9	0.081333899577
C2	H9	0.91072023909

C3	H9	0.0079103055535
C4	H9	0.00099004615562
H5	H9	0.011359181933
H6	H9	0.00090003630105
C7	H9	0.040662501171
H8	H9	0.041699647692
O1	O1	0.012582125783
C2	O1	0.043267843782
C3	O1	0.0015053541512
C4	O1	0.00030801386847
H5	O1	8.2887857972e-05
H6	O1	8.2885291113e-05
C7	O1	0.96713950608
H8	O1	0.003699503079
H9	O1	0.0036994163443
O1	H11	0.012030650834
C2	H11	0.040432291659
C3	H11	0.00048990150618
C4	H11	6.5842255947e-05
H5	H11	4.9486258392e-05
H6	H11	0.00043828344597
C7	H11	0.96142501585
H8	H11	0.010875454744
H9	H11	0.0039184564946
O1	H11	0.042226996816
O1	H12	0.012032933849
C2	H12	0.040465800758
C3	H12	0.00048970373145
C4	H12	6.5834578563e-05
H5	H12	0.0004383056084
H6	H12	4.947855541e-05
C7	H12	0.96139672137
H8	H12	0.003918521723
H9	H12	0.010875427101
O1	H12	0.042227165058
H11	H12	0.041797772264
O1	H13	0.012583587667
C2	H13	0.0015056500651
C3	H13	0.043276367394
C4	H13	0.96700613478
H5	H13	0.003697157414
H6	H13	0.0036971066402
C7	H13	0.00030807601134
H8	H13	8.2928301495e-05
H9	H13	8.2927809334e-05
O1	H13	0.00013524716241
H11	H13	1.6731705291e-05
H12	H13	1.6731756352e-05

O1	H14	0.012038909871
C2	H14	0.00049028663704
C3	H14	0.040520392049
C4	H14	0.9613832505
H5	H14	0.010877457907
H6	H14	0.0039175197004
C7	H14	6.5861858376e-05
H8	H14	4.9480623784e-05
H9	H14	0.00043834258491
O1	H14	1.6734190902e-05
H11	H14	4.5869375118e-06
H12	H14	2.402996618e-05
H13	H14	0.04222877206
O1	H15	0.012036269004
C2	H15	0.00048957188224
C3	H15	0.040456673783
C4	H15	0.96138008022
H5	H15	0.0039176561733
H6	H15	0.010877392903
C7	H15	6.5863932102e-05
H8	H15	0.00043834732297
H9	H15	4.947793955e-05
O1	H15	1.6734148634e-05
H11	H15	2.4030011334e-05
H12	H15	4.5869029627e-06
H13	H15	0.04222859438
H14	H15	0.041797219424

## DIMETHYL ETHER



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	C2	0.80976507563
O1	C3	0.80978686979
C2	C3	0.026194740651
O1	H4	0.071409095931
C2	H4	0.0081005858252
C3	H4	0.92970284766
O1	H5	0.082047373033
C2	H5	0.0077486947139
C3	H5	0.92402263088
H4	H5	0.039455614514
O1	H6	0.08197664828
C2	H6	0.0077529130894
C3	H6	0.92400370661
H4	H6	0.039455314555
H5	H6	0.042757983036
O1	H7	0.071404699244
C2	H7	0.92976845812
C3	H7	0.0081014410814
H4	H7	0.0018244061061
H5	H7	0.00087158649129
H6	H7	0.00087156099614
O1	H8	0.081964332222
C2	H8	0.9240086477
C3	H8	0.0077570867882
H4	H8	0.00087164798931
H5	H8	0.00086825154669
H6	H8	0.0099781985026
H7	H8	0.039469385094
O1	H9	0.082031991903
C2	H9	0.92399391499

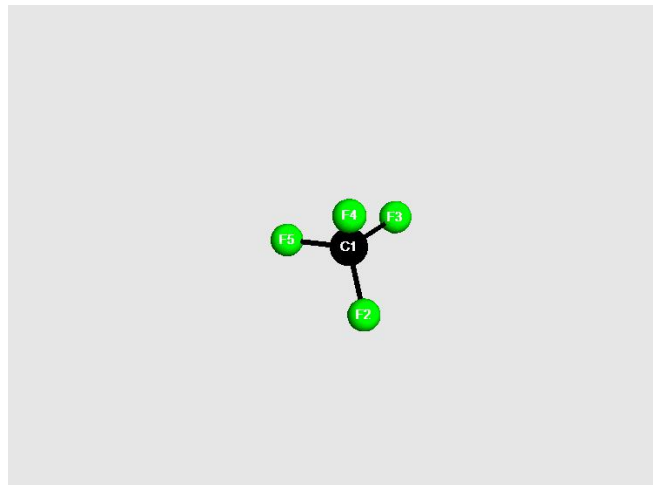
C3	H9	0.0077643228232
H4	H9	0.00087158545764
H5	H9	0.0099783586069
H6	H9	0.00086820010891
H7	H9	0.039469367302
H8	H9	0.042771070662

#### CCSD

Atom A	Atom B	Delocalization index
O1	C2	0.77170076661
O1	C3	0.77182249889
C2	C3	0.029313878427
O1	H4	0.052263457408
C2	H4	0.0072984283391
C3	H4	0.80496270494
O1	H5	0.06073945413
C2	H5	0.0081398834681
C3	H5	0.79694338001
H4	H5	0.030451236925
O1	H6	0.060654599084
C2	H6	0.0081469774631
C3	H6	0.79696134326
H4	H6	0.030450869403
H5	H6	0.033265466395
O1	H7	0.052261101493
C2	H7	0.80484255537
C3	H7	0.0073006436045
H4	H7	0.0017879538162
H5	H7	0.00082874703448
H6	H7	0.00082873928119
O1	H8	0.060651425175
C2	H8	0.79697809893
C3	H8	0.0081580106808
H4	H8	0.00082880761059
H5	H8	0.00096819283965
H6	H8	0.011711973835
H7	H8	0.0304509392
O1	H9	0.060733213896
C2	H9	0.79693685334
C3	H9	0.0081533973569
H4	H9	0.0008287590478
H5	H9	0.011711927457
H6	H9	0.00096812342216
H7	H9	0.030450829137
H8	H9	0.033265391935

# HALOALKANES

## CARBON TETRAFLUORIDE



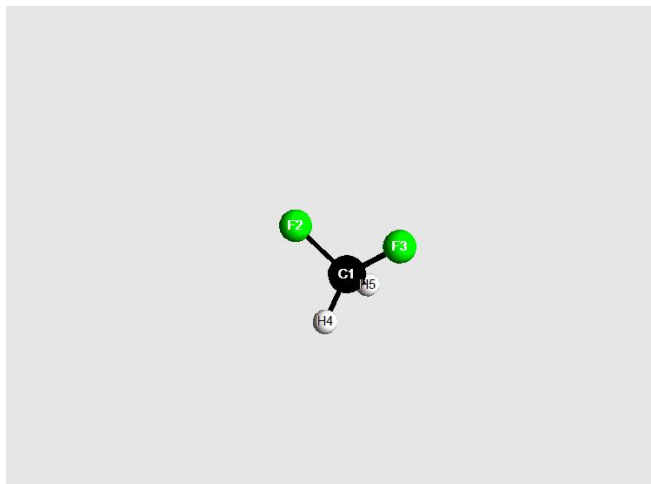
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	F2	0.46263456844
C1	F3	0.46288235698
F2	F3	0.17709605781
C1	F4	0.4629095603
F2	F4	0.17709517762
F3	F4	0.17709947035
C1	F5	0.46349482168
F2	F5	0.17709563626
F3	F5	0.17709603509
F4	F5	0.17709558756

### CCSD

Atom A	Atom B	Delocalization index
C1	F2	0.51245827221
C1	F3	0.51256985196
F2	F3	0.14408669362
C1	F4	0.51185718452
F2	F4	0.14408732773
F3	F4	0.14408828987
C1	F5	0.5119439795
F2	F5	0.14408752425
F3	F5	0.14408883666
F4	F5	0.14408772725

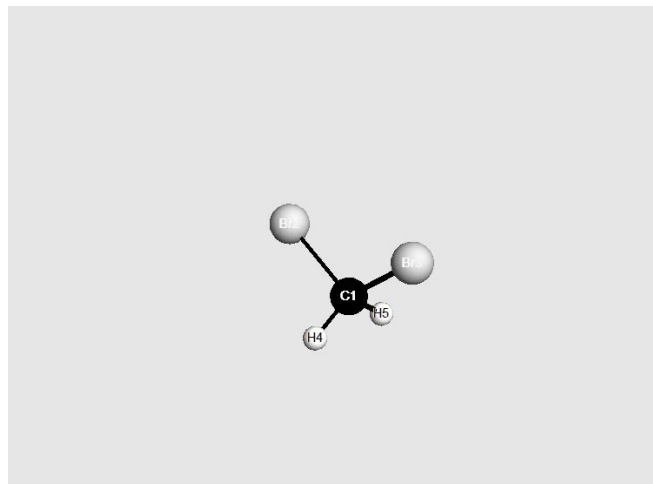
## DIFLUOROMETHANE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	F2	0.65631797883
C1	F3	0.65634896516
F2	F3	0.16867621951
C1	H4	0.88431253161
F2	H4	0.072155769785
F3	H4	0.072119495231
C1	H5	0.88426788966
F2	H5	0.072155590937
F3	H5	0.072119330039
H4	H5	0.030986661182

## DIBROMOMETHANE

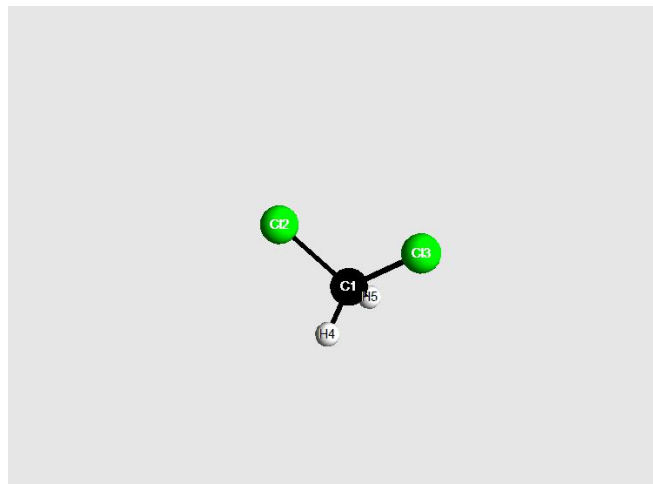


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	Br2	1.1085189935
C1	Br3	1.1084620436
Br2	Br3	0.1485581641
C1	H4	0.94130420754
Br2	H4	0.057686771888
Br3	H4	0.057686119338
C1	H5	0.941281528
Br2	H5	0.057686801358
Br3	H5	0.05768629047
H4	H5	0.027466666926



## DICHLOROMETHANE

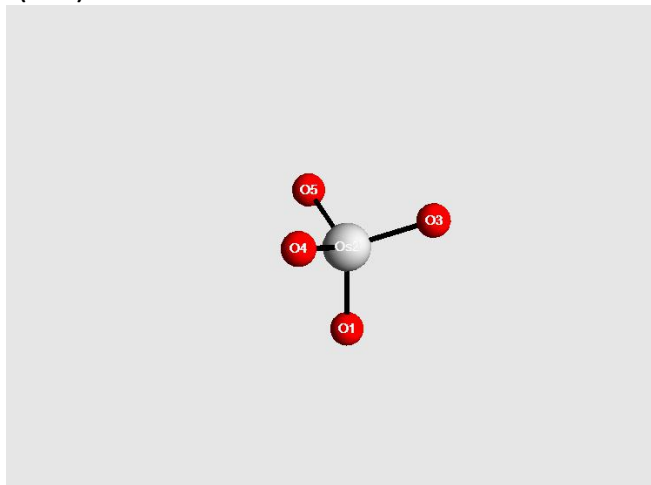


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	Cl2	1.0647297064
C1	Cl3	1.0647446424
Cl2	Cl3	0.15384385383
C1	H4	0.92677841171
Cl2	H4	0.062244366564
Cl3	H4	0.062244258301
C1	H5	0.92678697357
Cl2	H5	0.062244206574
Cl3	H5	0.062244119835
H4	H5	0.027120075493

# INORGANICS

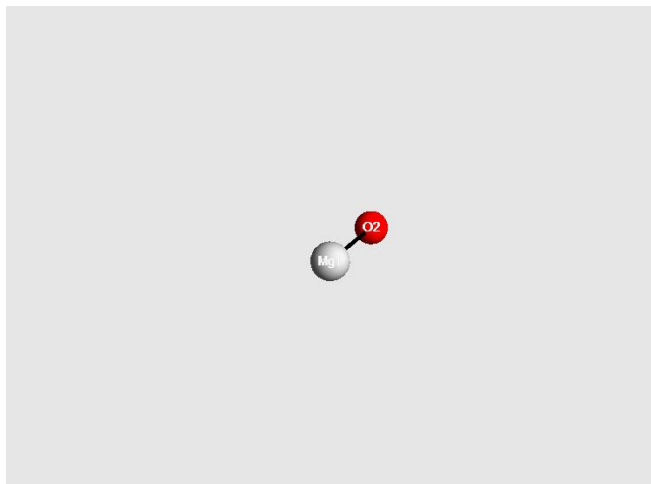
## OSMIUM OXIDE (VIII)



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	Os2	1.6940155477
O1	O3	0.18877832535
Os2	O3	1.6940386718
O1	O4	0.18877822738
Os2	O4	1.6939738897
O3	O4	0.18877826793
O1	O5	0.18877825758
Os2	O5	1.6939637201
O3	O5	0.18877842227
O4	O5	0.18877828669

## MAGNESIUM OXIDE



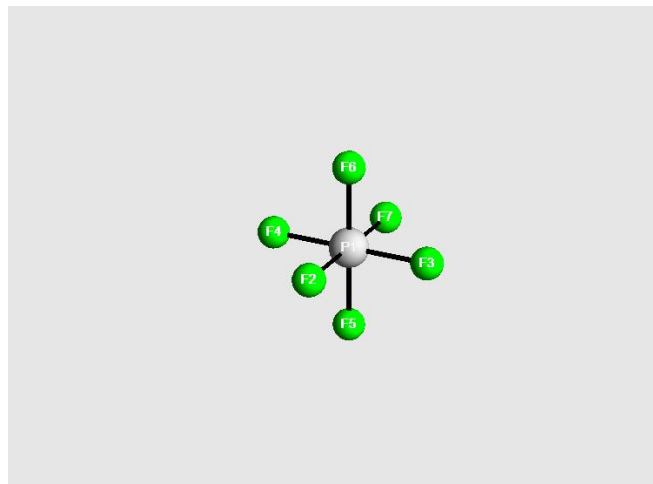
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
Mg1	O2	1.0084532771

### CCSD

Atom A	Atom B	Delocalization index
Mg1	O2	0.84122171716

## HEXAFLUOROPHOSPHATE ANION



### HARTREE-FOCK

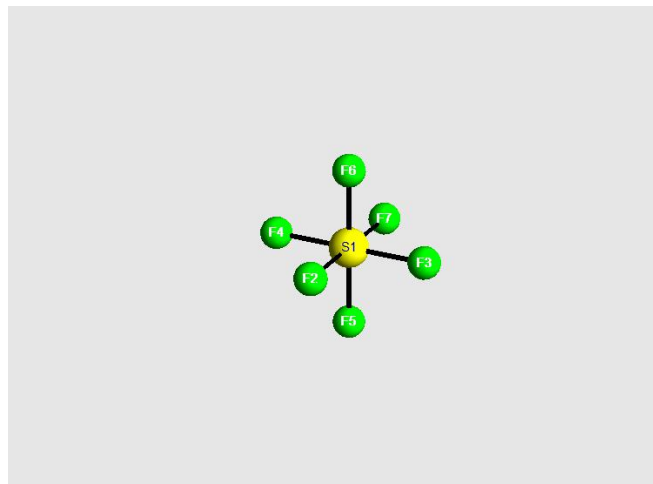
Atom A	Atom B	Delocalization index
P1	F2	0.29635030296
P1	F3	0.29584529262
F2	F3	0.14372342302
P1	F4	0.29584772367
F2	F4	0.14372765911
F3	F4	0.0027887530299
P1	F5	0.29584839252
F2	F5	0.14372396541
F3	F5	0.14372366554
F4	F5	0.14372748786
P1	F6	0.29584649233
F2	F6	0.14373158177
F3	F6	0.14372624115
F4	F6	0.14372047786
F5	F6	0.0027888462576
P1	F7	0.29634664718
F2	F7	0.0027889868964
F3	F7	0.14372978375
F4	F7	0.1437217869
F5	F7	0.14373266101
F6	F7	0.14372660307

### CCSD

Atom A	Atom B	Delocalization index
P1	F2	0.31498318122
P1	F3	0.31444929451
F2	F3	0.12981489746
P1	F4	0.31444931234
F2	F4	0.12981871441
F3	F4	0.0029746806511

P1	F5	0.31445095926
F2	F5	0.12981739278
F3	F5	0.12981337882
F4	F5	0.12981797922
P1	F6	0.31445085778
F2	F6	0.12981968944
F3	F6	0.12981757096
F4	F6	0.12981400205
F5	F6	0.0029748095536
P1	F7	0.3149866431
F2	F7	0.0029749996714
F3	F7	0.12981874248
F4	F7	0.12981742223
F5	F7	0.12982190682
F6	F7	0.12981739214

## SULFUR HEXAFLUORIDE



### HARTREE-FOCK

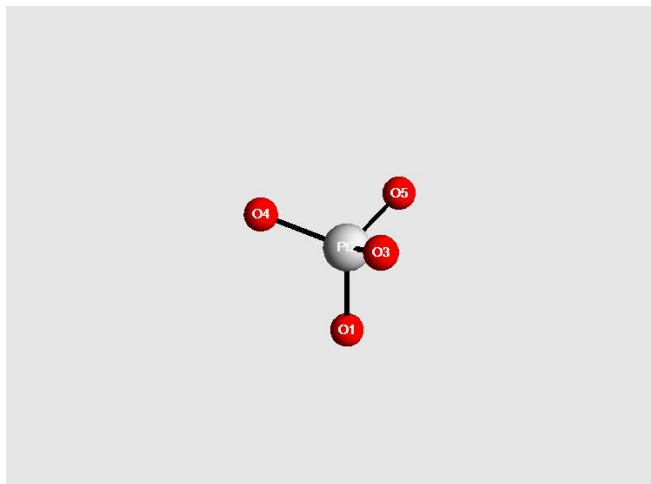
Atom A	Atom B	Delocalization index
S1	F2	0.46354179029
S1	F3	0.46294254816
F2	F3	0.15754152367
S1	F4	0.46295149484
F2	F4	0.15754452879
F3	F4	0.0052777142439
S1	F5	0.4629456623
F2	F5	0.15754628121
F3	F5	0.15753813619
F4	F5	0.15754197501
S1	F6	0.46294816264
F2	F6	0.15754256146
F3	F6	0.15754661185
F4	F6	0.15754514035
F5	F6	0.0052777760927
S1	F7	0.46354431421
F2	F7	0.0052778638425
F3	F7	0.15754393638
F4	F7	0.15754122776
F5	F7	0.15754410401
F6	F7	0.1575446276

### CCSD

Atom A	Atom B	Delocalization index
S1	F2	0.49835965102
S1	F3	0.49776634019
F2	F3	0.12870512666
S1	F4	0.49776758304
F2	F4	0.12870535167
F3	F4	0.0046026099764

S1	F5	0.49776586742
F2	F5	0.12870567317
F3	F5	0.12870431692
F4	F5	0.12870379055
S1	F6	0.49776529339
F2	F6	0.12870519839
F3	F6	0.12870417219
F4	F6	0.128703206
F5	F6	0.0046026587998
S1	F7	0.49835673477
F2	F7	0.0046027573167
F3	F7	0.12870420574
F4	F7	0.12870200949
F5	F7	0.12870454126
F6	F7	0.1287039509

## PLATINATE (VII) ANION

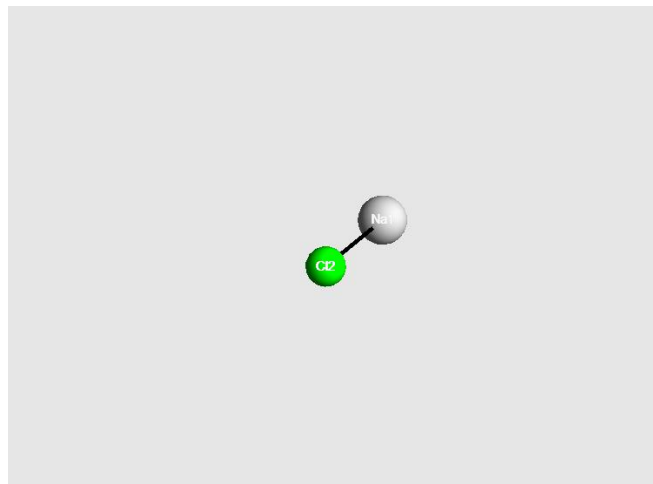


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	Pt2	1.6785221589
O1	O3	0.31858693526
Pt2	O3	1.6785214043
O1	O4	0.31858724186
Pt2	O4	1.6784957409
O3	O4	0.3185881796
O1	O5	0.31858712241
Pt2	O5	1.678504162
O3	O5	0.31858797748
O4	O5	0.31859037431



## SODIUM CHLORIDE



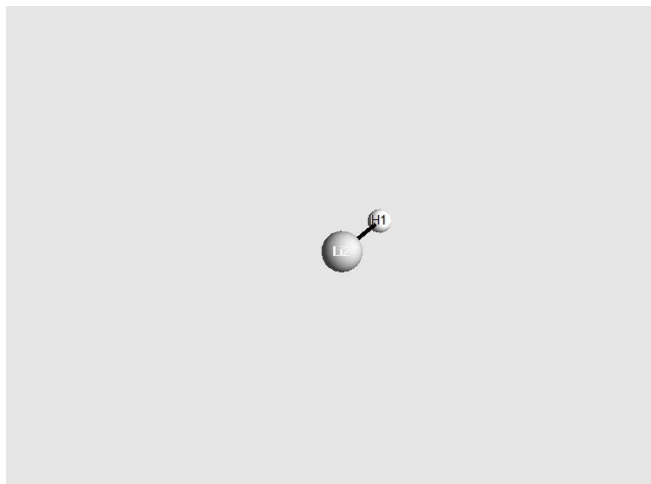
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
Na1	Cl2	0.21571872708

### CCSD

Atom A	Atom B	Delocalization index
Na1	Cl2	0.22182137578

## LITHIUM HYDRIDE



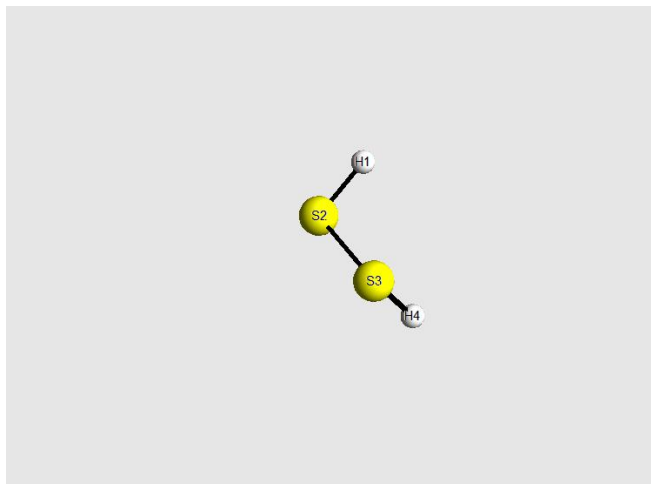
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	Li2	0.19251326055

### CCSD

Atom A	Atom B	Delocalization index
H1	Li2	0.19881788123

## HYDROGEN DISULFIDE



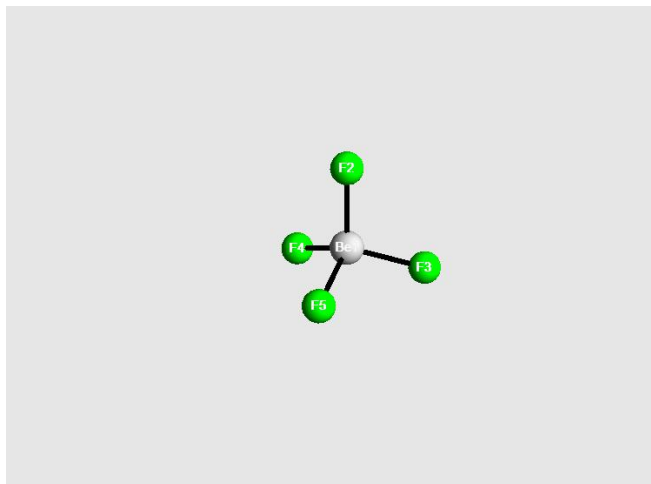
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	S2	1.1183518991
H1	S3	0.071030764268
S2	S3	1.286936101
H1	H4	0.0032718605291
S2	H4	0.071031938658
S3	H4	1.1183136072

### CCSD

Atom A	Atom B	Delocalization index
H1	S2	0.93472466101
H1	S3	0.055216251071
S2	S3	1.0247151309
H1	H4	0.0027599645372
S2	H4	0.055217608208
S3	H4	0.93461844082

## TETRAFLUOROBERYLLATE ANION



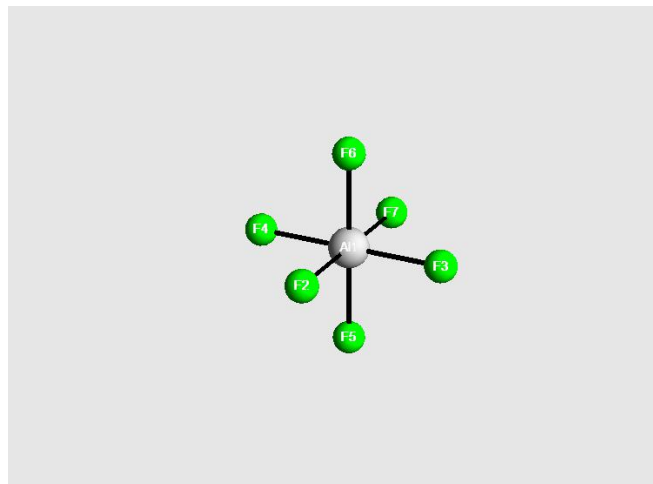
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
Be1	F2	0.10944091762
Be1	F3	0.10954409622
F2	F3	0.08831942241
Be1	F4	0.10932682592
F2	F4	0.088319322537
F3	F4	0.088318366091
Be1	F5	0.10944913541
F2	F5	0.088318937906
F3	F5	0.088317965429
F4	F5	0.088319921018

### CCSD

Atom A	Atom B	Delocalization index
Be1	F2	0.11431914618
Be1	F3	0.11444638201
F2	F3	0.092265132744
Be1	F4	0.11416780239
F2	F4	0.09226408373
F3	F4	0.092263960497
Be1	F5	0.11432204044
F2	F5	0.092263807077
F3	F5	0.09226295118
F4	F5	0.092264675734

## HEXAFLUOROALUMINATE ANION



### HARTREE-FOCK

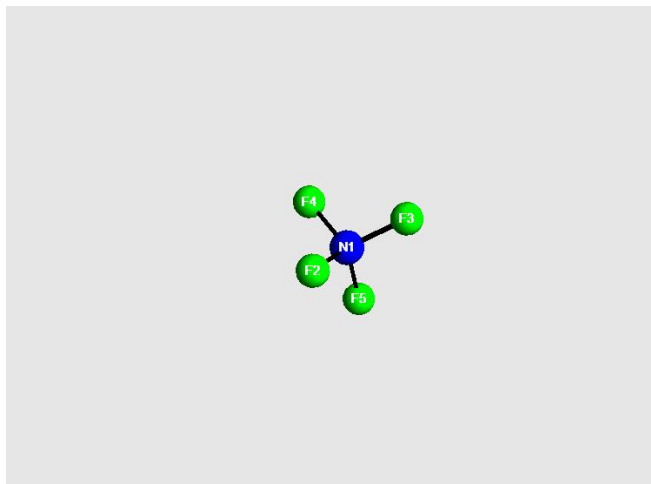
Atom A	Atom B	Delocalization index
Al1	F2	0.125338435
Al1	F3	0.12548698289
F2	F3	0.076036844429
Al1	F4	0.12548036688
F2	F4	0.076054290183
F3	F4	0.0011682540487
Al1	F5	0.12548870845
F2	F5	0.076043566567
F3	F5	0.076033220945
F4	F5	0.076056603308
Al1	F6	0.12548042402
F2	F6	0.076061847723
F3	F6	0.076056716426
F4	F6	0.076033297379
F5	F6	0.0011683352355
Al1	F7	0.12533752809
F2	F7	0.001168449059
F3	F7	0.076054712562
F4	F7	0.076037381402
F5	F7	0.076061771597
F6	F7	0.076042344999

### CCSD

Atom A	Atom B	Delocalization index
Al1	F2	0.12925369659
Al1	F3	0.12943593352
F2	F3	0.078551367411
Al1	F4	0.12942775962
F2	F4	0.078567577335
F3	F4	0.0019970032325

A11	F5	0.12943730732
F2	F5	0.078557348078
F3	F5	0.078546988095
F4	F5	0.078566695236
A11	F6	0.12942625911
F2	F6	0.07857446711
F3	F6	0.078568258752
F4	F6	0.078546689564
F5	F6	0.0019971996264
A11	F7	0.12925031536
F2	F7	0.0019974687421
F3	F7	0.078568251504
F4	F7	0.078549899324
F5	F7	0.078574671366
F6	F7	0.078556419436

## TETRAFLUOROAMMONIUM



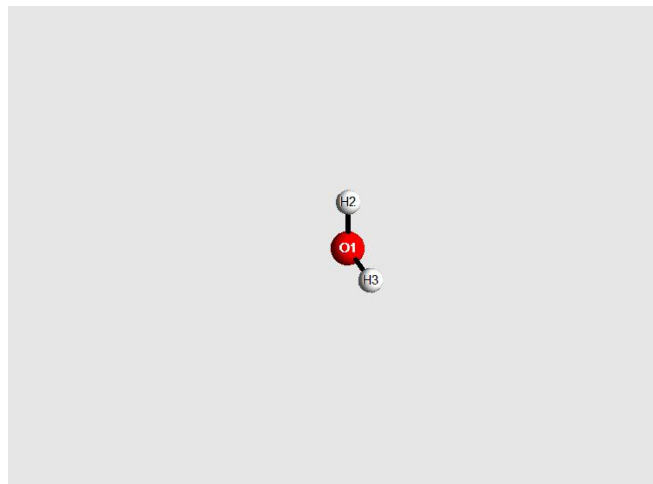
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	F2	1.0617882351
N1	F3	1.0618045525
F2	F3	0.11959838554
N1	F4	1.0613558455
F2	F4	0.11959805282
F3	F4	0.11960253997
N1	F5	1.0613591438
F2	F5	0.11959840154
F3	F5	0.11960217464
F4	F5	0.11960149873

### CCSD

Atom A	Atom B	Delocalization index
N1	F2	0.87671004814
N1	F3	0.87670927529
F2	F3	0.09813905107
N1	F4	0.8762865466
F2	F4	0.09813944584
F3	F4	0.0981382739
N1	F5	0.8762788101
F2	F5	0.098138975933
F3	F5	0.098139298989
F4	F5	0.098140058428

## WATER



### HARTREE-FOCK

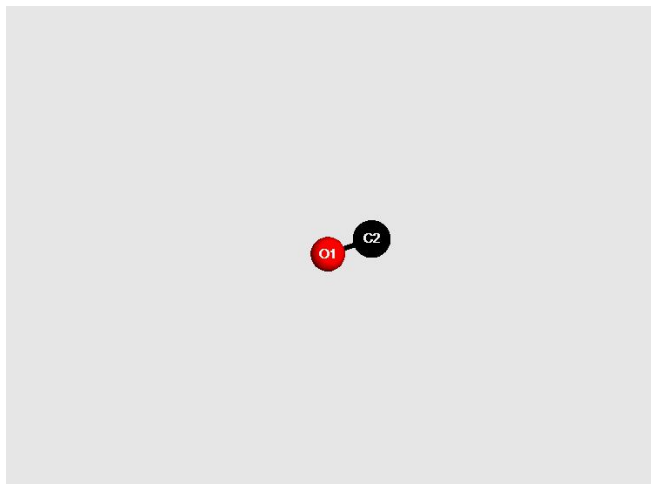
Atom A	Atom B	Delocalization index
O1	H2	0.61649611339
O1	H3	0.61649789234
H2	H3	0.0067544084164

### CCSD

Atom A	Atom B	Delocalization index
O1	H2	0.61466493859
O1	H3	0.61466623586
H2	H3	0.0087446804635



## CARBON MONOXIDE



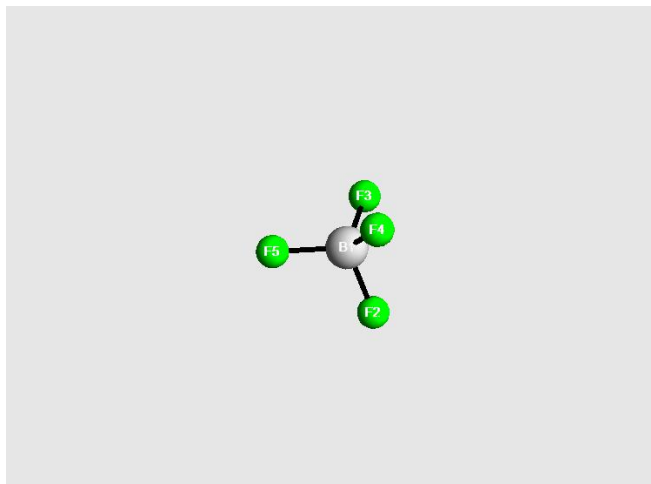
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	C2	1.5732996512

### CCSD

Atom A	Atom B	Delocalization index
O1	C2	1.4525188951

## TETRAFLUOROBORATE ANION



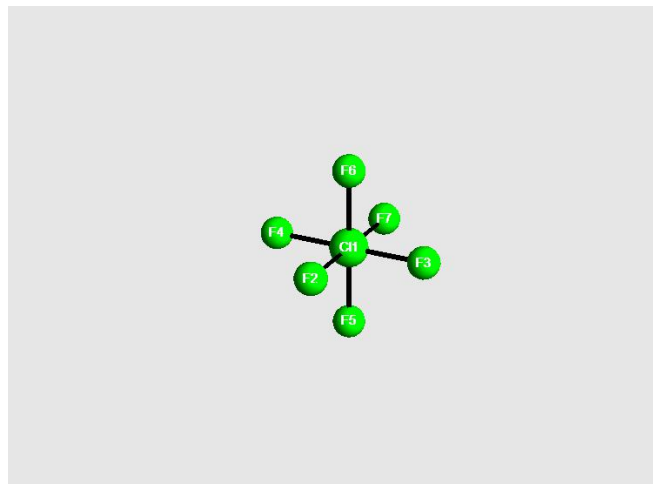
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
B1	F2	0.21086019475
B1	F3	0.2111575468
F2	F3	0.15245290867
B1	F4	0.21031565541
F2	F4	0.152453872
F3	F4	0.15245413703
B1	F5	0.21067184241
F2	F5	0.15245367321
F3	F5	0.1524517972
F4	F5	0.15245396744

### CCSD

Atom A	Atom B	Delocalization index
B1	F2	0.22768175454
B1	F3	0.22797045856
F2	F3	0.14428975817
B1	F4	0.2270544957
F2	F4	0.14429091339
F3	F4	0.14429070137
B1	F5	0.22738787218
F2	F5	0.14429170002
F3	F5	0.14428975334
F4	F5	0.14429021221

## CHLORINE HEXAFLUORIDE ANION



### HARTREE-FOCK

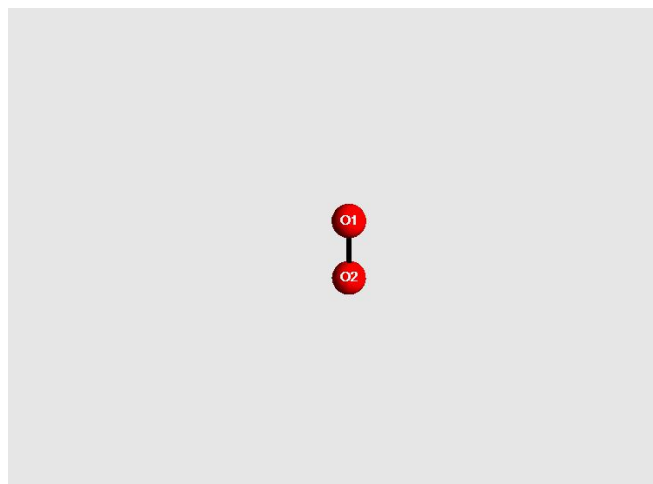
Atom A	Atom B	Delocalization index
Cl1	F2	0.80082537293
Cl1	F3	0.80029955443
F2	F3	0.1378632739
Cl1	F4	0.80030458526
F2	F4	0.13786189719
F3	F4	0.011686478131
Cl1	F5	0.80030264271
F2	F5	0.13786135211
F3	F5	0.13786290109
F4	F5	0.13786056463
Cl1	F6	0.80030399718
F2	F6	0.13786536799
F3	F6	0.13786377988
F4	F6	0.13786337751
F5	F6	0.011686540742
Cl1	F7	0.80082505418
F2	F7	0.011686598651
F3	F7	0.13786317316
F4	F7	0.13786301183
F5	F7	0.13786444466
F6	F7	0.1378633541

### CCSD

Atom A	Atom B	Delocalization index
Cl1	F2	0.71661977076
Cl1	F3	0.71613405241
F2	F3	0.10514763593
Cl1	F4	0.71613530861
F2	F4	0.10514905034
F3	F4	0.0092849450336

Cl1	F5	0.71613636592
F2	F5	0.1051504841
F3	F5	0.10514909421
F4	F5	0.10514906406
Cl1	F6	0.71613308671
F2	F6	0.10514951713
F3	F6	0.10514860438
F4	F6	0.10514866453
F5	F6	0.0092850032819
Cl1	F7	0.71661776308
F2	F7	0.0092850631614
F3	F7	0.10514813267
F4	F7	0.10514926794
F5	F7	0.10514959839
F6	F7	0.10514879278

## OXYGEN



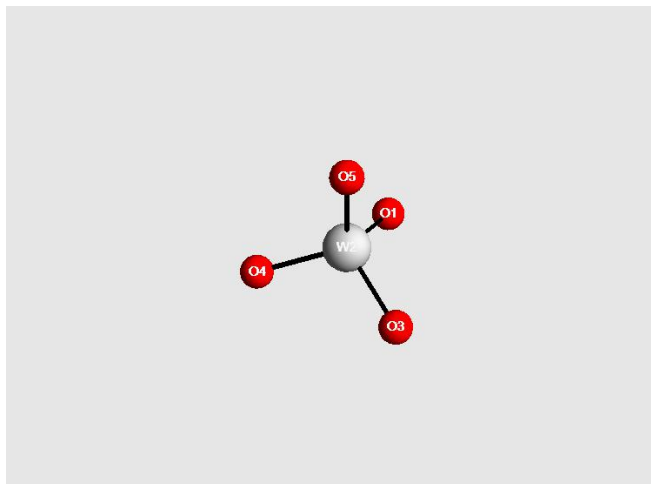
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	O2	2.2715486647

### CCSD

Atom A	Atom B	Delocalization index
O1	O2	1.6147737861

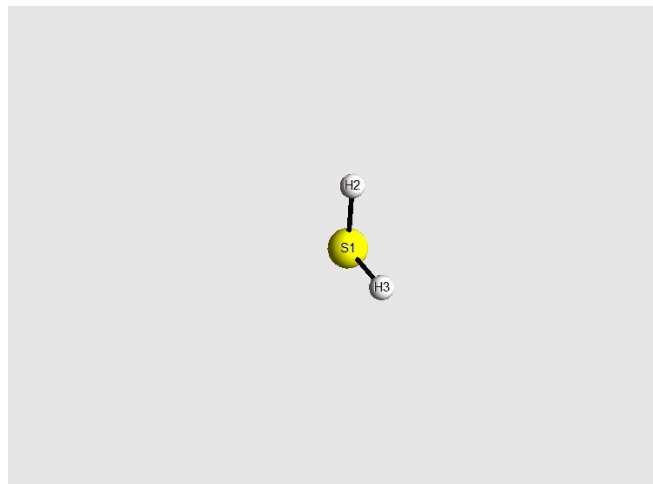
## ORTHOTUNGSTATE ANION



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	W2	1.5678940748
O1	O3	0.078935966268
W2	O3	1.5678850354
O1	O4	0.078935895391
W2	O4	1.5678937791
O3	O4	0.0789357329
O1	O5	0.078935998382
W2	O5	1.5678829818
O3	O5	0.078935842738
O4	O5	0.078935759329

## HYDROGEN SULFIDE



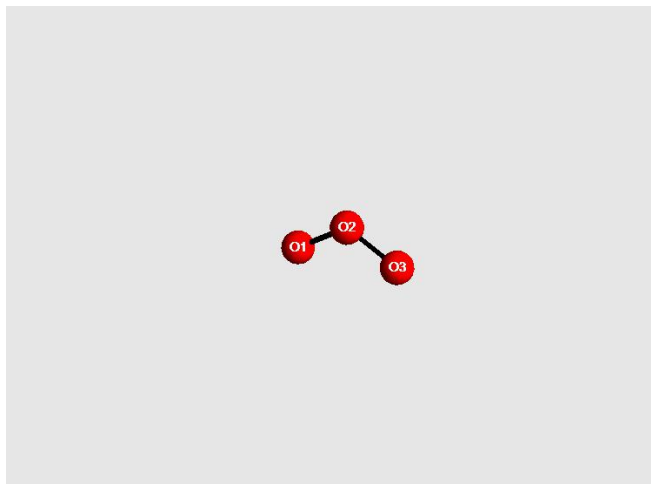
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
S1	H2	1.1422431297
S1	H3	1.1422414432
H2	H3	0.055611114221

### CCSD

Atom A	Atom B	Delocalization index
S1	H2	0.95510496958
S1	H3	0.95510613128
H2	H3	0.043339705927

## OZONE



### HARTREE-FOCK

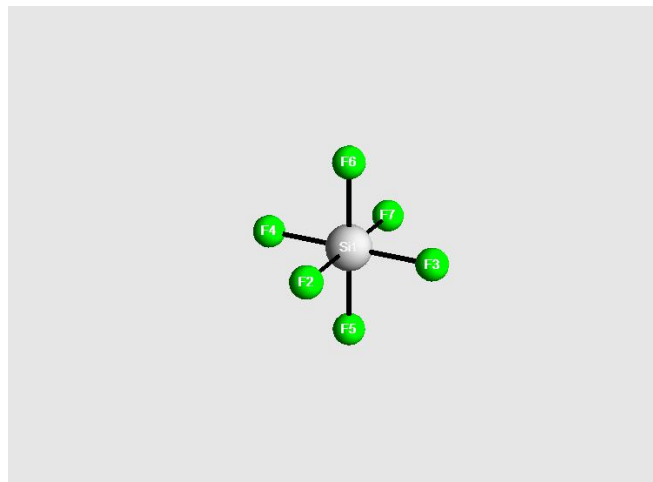
Atom A	Atom B	Delocalization index
O1	O2	1.7245550924
O1	O3	0.47895663764
O2	O3	1.7244070734

### CCSD

Atom A	Atom B	Delocalization index
O1	O2	1.259069141
O1	O3	0.33337892095
O2	O3	1.2590653644



## HEXAFLUROSILICATE ANION



### HARTREE-FOCK

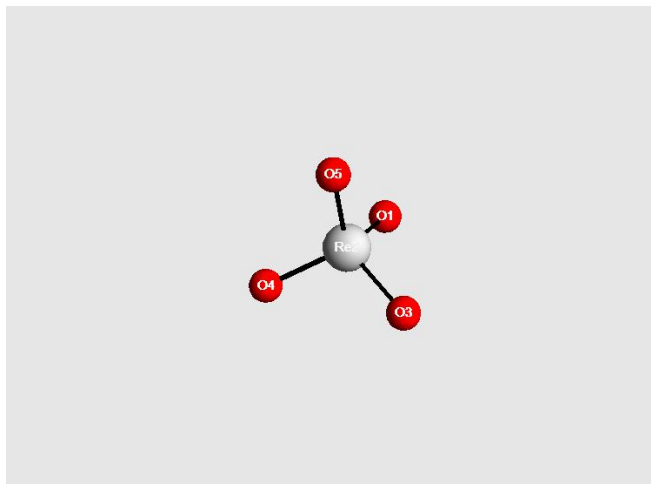
Atom A	Atom B	Delocalization index
Si1	F2	0.19704894773
Si1	F3	0.19652974887
F2	F3	0.11374966592
Si1	F4	0.19652709227
F2	F4	0.11376435887
F3	F4	0.001581736976
Si1	F5	0.19652966508
F2	F5	0.11375391926
F3	F5	0.11374611144
F4	F5	0.11376285811
Si1	F6	0.19652895354
F2	F6	0.11376822842
F3	F6	0.11376111273
F4	F6	0.11374764672
F5	F6	0.0015818307451
Si1	F7	0.19704919195
F2	F7	0.0015819941682
F3	F7	0.11376314077
F4	F7	0.11375030269
F5	F7	0.11376968912
F6	F7	0.11375411789

### CCSD

Atom A	Atom B	Delocalization index
Si1	F2	0.20499289375
Si1	F3	0.20437414611
F2	F3	0.10988613693
Si1	F4	0.20437479991
F2	F4	0.10989651094
F3	F4	0.0020930273073

Si1	F5	0.20437147152
F2	F5	0.10988877949
F3	F5	0.10988276946
F4	F5	0.10989297635
Si1	F6	0.20437655901
F2	F6	0.10990062407
F3	F6	0.10989427205
F4	F6	0.1098836902
F5	F6	0.0020931797552
Si1	F7	0.20499069731
F2	F7	0.0020934329893
F3	F7	0.1098948503
F4	F7	0.10988591284
F5	F7	0.10989897707
F6	F7	0.10988848463

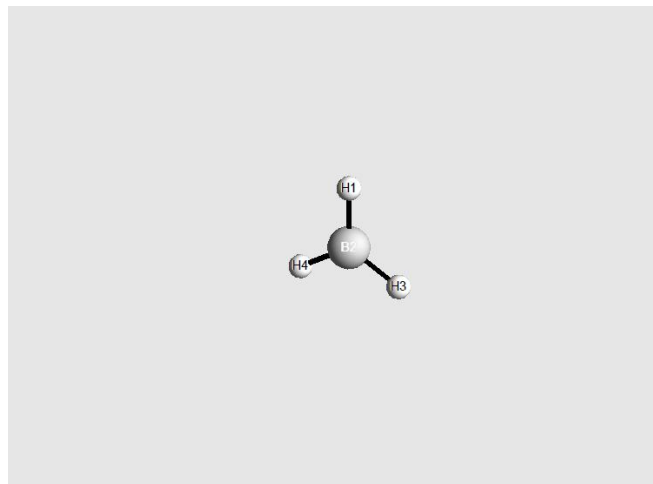
## RENATE (VII) ANION



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
O1	Re2	1.5151975888
O1	O3	0.14476073062
Re2	O3	1.5152956854
O1	O4	0.14476086593
Re2	O4	1.5152667978
O3	O4	0.14476156728
O1	O5	0.14476058396
Re2	O5	1.5152020576
O3	O5	0.14476131749
O4	O5	0.14476119682

## BORANE



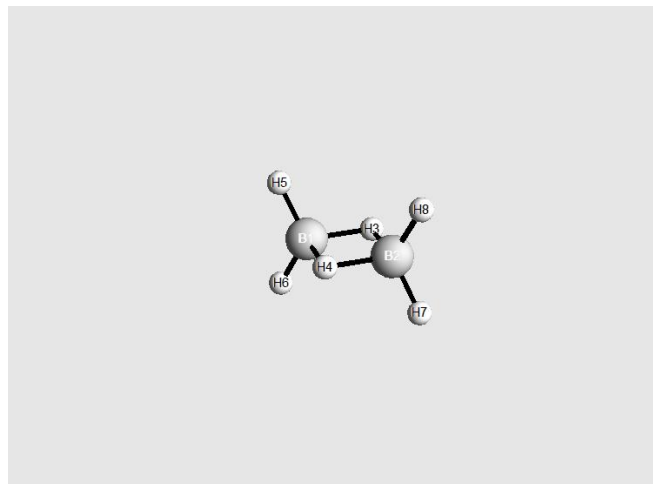
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	B2	0.50804812759
H1	H3	0.14439027054
B2	H3	0.50806998316
H1	H4	0.14439028027
B2	H4	0.50804105518
H3	H4	0.1443900561

### CCSD

Atom A	Atom B	Delocalization index
H1	B2	0.52168726284
H1	H3	0.11288497929
B2	H3	0.52171319956
H1	H4	0.11288474045
B2	H4	0.52169323635
H3	H4	0.11288499102

## DIBORANE



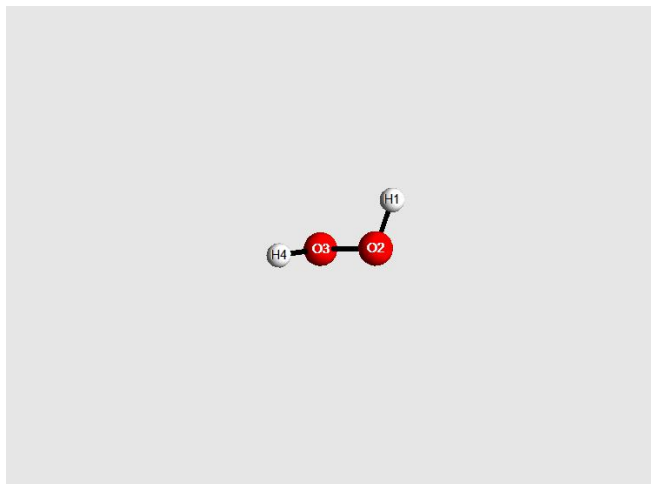
## HARTREE-FOCK

Atom A	Atom B	Delocalization index
B1	B2	0.05528880321
B1	H3	0.28005992914
B2	H3	0.27988107897
B1	H4	0.27988611353
B2	H4	0.28005704616
H3	H4	0.21826272944
B1	H5	0.49533419712
B2	H5	0.018372317818
H3	H5	0.11091106821
H4	H5	0.11090505309
B1	H6	0.49554541854
B2	H6	0.018359918882
H3	H6	0.11090901814
H4	H6	0.11090268424
H5	H6	0.12548099759
B1	H7	0.018372682826
B2	H7	0.49532418103
H3	H7	0.11090334055
H4	H7	0.1109092025
H5	H7	0.014345358039
H6	H7	0.010660996227
B1	H8	0.018360745308
B2	H8	0.49554279295
H3	H8	0.1109047842
H4	H8	0.1109114073
H5	H8	0.010671409885
H6	H8	0.014345288367
H7	H8	0.12548176762

## CCSD

Atom A	Atom B	Delocalization index
B1	B2	0.059214205647
B1	H3	0.30413168793
B2	H3	0.30402703571
B1	H4	0.30403165076
B2	H4	0.30413198306
H3	H4	0.16706044741
B1	H5	0.51196266052
B2	H5	0.015982436906
H3	H5	0.08830368901
H4	H5	0.088300505912
B1	H6	0.51153095107
B2	H6	0.016020504402
H3	H6	0.088304425448
H4	H6	0.088296737006
H5	H6	0.095146568579
B1	H7	0.015981754035
B2	H7	0.5119596988
H3	H7	0.08829939325
H4	H7	0.088302892391
H5	H7	0.011573327513
H6	H7	0.0094236867201
B1	H8	0.016022316117
B2	H8	0.51152604038
H3	H8	0.088298004173
H4	H8	0.088306121759
H5	H8	0.0094311911289
H6	H8	0.011573324224
H7	H8	0.095147007733

## HYDROGEN PEROXIDE



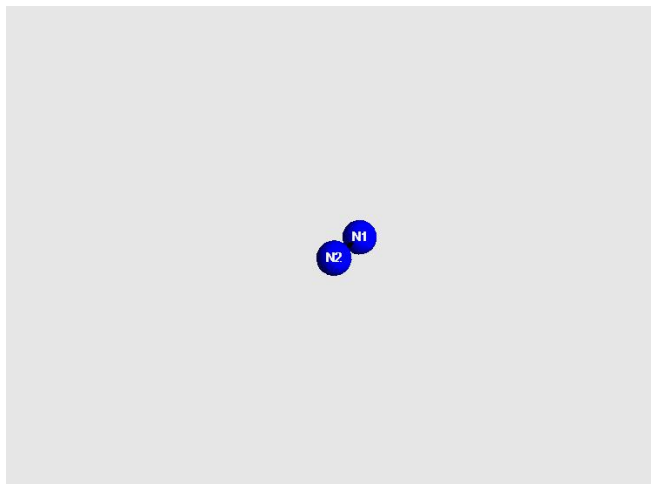
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	O2	0.5834609473
H1	O3	0.023694352891
O2	O3	1.2976200238
H1	H4	0.00067473192968
O2	H4	0.023694414929
O3	H4	0.58347996818

### CCSD

Atom A	Atom B	Delocalization index
H1	O2	0.58390816007
H1	O3	0.022826427843
O2	O3	0.97176955194
H1	H4	0.00083660925438
O2	H4	0.022824665297
O3	H4	0.58395175273

## NITROGEN



### HARTREE-FOCK

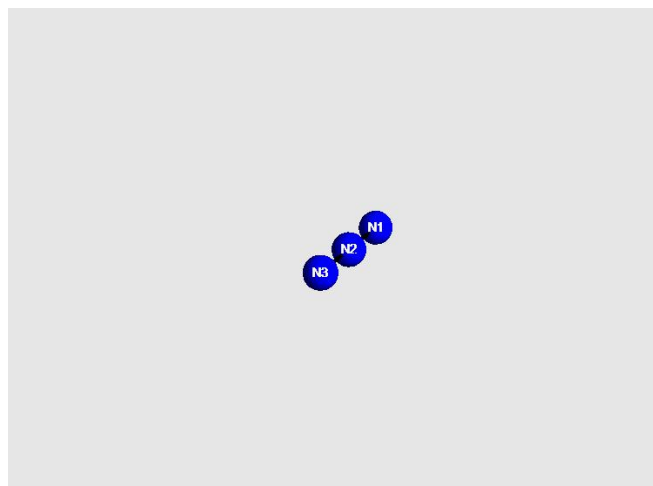
Atom A	Atom B	Delocalization index
N1	N2	3.0420751562

### CCSD

Atom A	Atom B	Delocalization index
N1	N2	2.3098417756



## AZIDE ANION



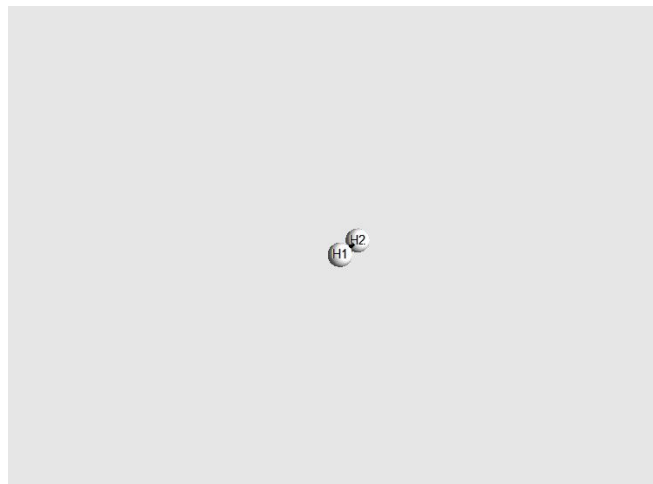
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	N2	2.1881437324
N1	N3	0.58520691369
N2	N3	2.1881345484

### CCSD

Atom A	Atom B	Delocalization index
N1	N2	2.1881439613
N1	N3	0.58520689603
N2	N3	2.1881347747

## HYDROGEN



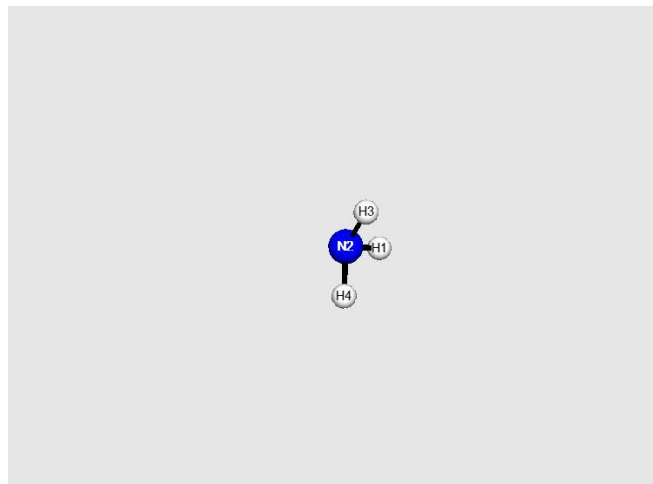
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
H1	H2	1.0000008336

### CCSD

Atom A	Atom B	Delocalization index
H1	H2	0.843945036

## AMMONIA



### HARTREE-FOCK

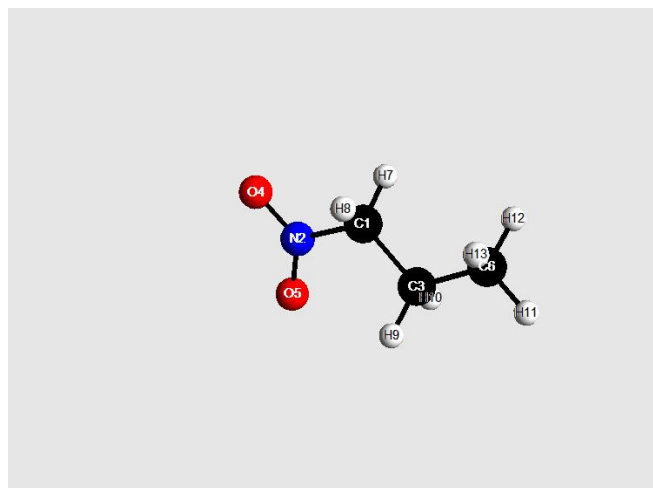
Atom A	Atom B	Delocalization index
H1	N2	0.89424468702
H1	H3	0.01857310355
N2	H3	0.8942575027
H1	H4	0.018573396162
N2	H4	0.89425214267
H3	H4	0.018574786535

### CCSD

Atom A	Atom B	Delocalization index
H1	N2	0.79196793572
H1	H3	0.018159647432
N2	H3	0.79196449804
H1	H4	0.01816000339
N2	H4	0.79196794872
H3	H4	0.018159926496

# NITRODERIVATIVES

## NITROPROPANE



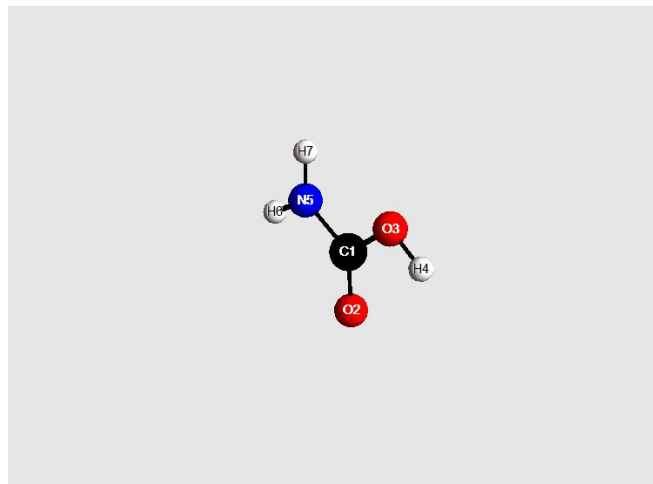
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	N2	0.74736870786
C1	C3	0.95736654352
N2	C3	0.042770558243
C1	O4	0.080528103717
N2	O4	1.6845890987
C3	O4	0.011519477892
C1	O5	0.067194896653
N2	O5	1.699928815
C3	O5	0.036058951085
O4	O5	0.32975115296
C1	C6	0.051607073252
N2	C6	0.0088352531091
C3	C6	0.97653015568
O4	C6	0.0020863597866
O5	C6	0.0041478206131
C1	H7	0.91640321503
N2	H7	0.058270654776
C3	H7	0.031144465785
O4	H7	0.018974610908
O5	H7	0.011943423946
C6	H7	0.006741505594
C1	H8	0.9162954596
N2	H8	0.058377798864
C3	H8	0.031152040741
O4	H8	0.018870430106
O5	H8	0.011942709122
C6	H8	0.0067301460789
H7	H8	0.032865923716

C1	H9	0.043841734735
N2	H9	0.003888030791
C3	H9	0.9426132808
O4	H9	0.0012872663758
O5	H9	0.016310237884
C6	H9	0.039149008155
H7	H9	0.0095932928728
H8	H9	0.0032144850706
C1	C1	0.043877498795
N2	C1	0.0039152218613
C3	C1	0.94276529085
O4	C1	0.0012867044363
O5	C1	0.016165824895
C6	C1	0.039163767161
H7	C1	0.0032073489526
H8	C1	0.0095991094223
H9	C1	0.038507684241
C1	H11	0.010434019203
N2	H11	0.0019165477959
C3	H11	0.042219759042
O4	H11	0.00067948361991
O5	H11	0.00021552816933
C6	H11	0.9641455172
H7	H11	0.00073993856699
H8	H11	0.0007390639373
H9	H11	0.0036401079767
C1	H11	0.0036402742349
C1	H12	0.0074747550717
N2	H12	0.00059873855424
C3	H12	0.042374609056
O4	H12	0.00015745310361
O5	H12	0.00063005207939
C6	H12	0.96355096396
H7	H12	0.0054874487507
H8	H12	0.00044809657646
H9	H12	0.010835369672
C1	H12	0.0034001603952
H11	H12	0.042754315632
C1	H13	0.0074699387868
N2	H13	0.0005998028996
C3	H13	0.042363798411
O4	H13	0.00015829146807
O5	H13	0.00062700048792
C6	H13	0.96355370442
H7	H13	0.00044835390718
H8	H13	0.0054823201458
H9	H13	0.0033985472411
C1	H13	0.010840387346

H11	H13	0.042754930272
H12	H13	0.043878620074

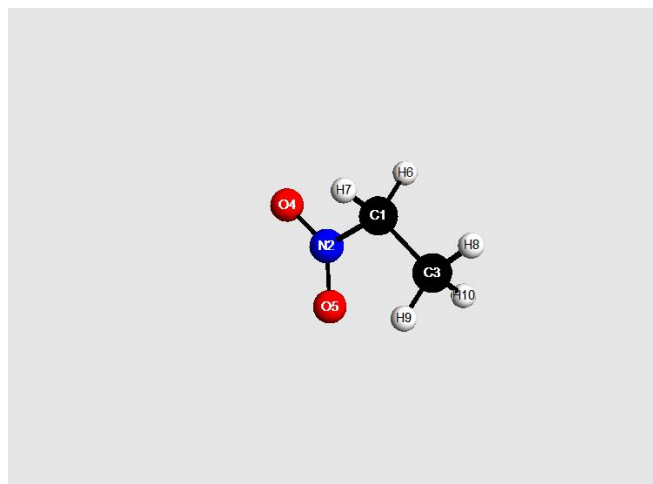
## NITROMETHANE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	O2	0.97062038722
C1	O3	0.64178217106
O2	O3	0.26858196811
C1	H4	0.0056886771034
O2	H4	0.0095763052142
O3	H4	0.53542061767
C1	N5	0.82899265525
O2	N5	0.24333183968
O3	N5	0.19174531656
H4	N5	0.0073468308687
C1	H6	0.012189387392
O2	H6	0.0081912664127
O3	H6	0.0093912161454
H4	H6	0.00096484883889
N5	H6	0.78762621503
C1	H7	0.012215541393
O2	H7	0.01321507604
O3	H7	0.008082704813
H4	H7	0.00020051892252
N5	H7	0.79195726086
H6	H7	0.014028019983

## NITROETHANE



### HARTREE-FOCK

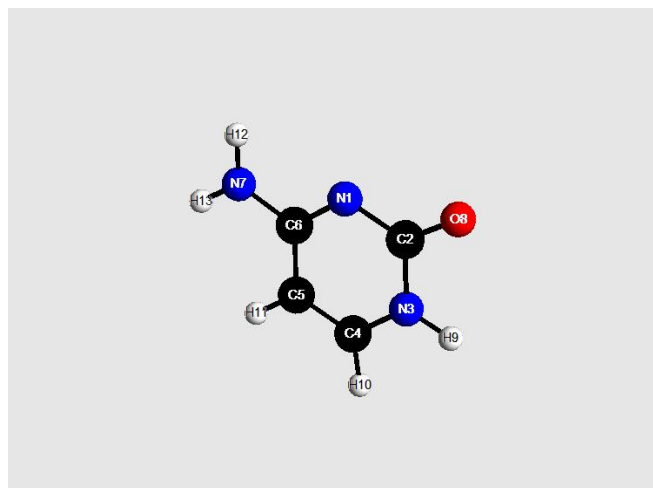
Atom A	Atom B	Delocalization index
C1	N2	0.74808305772
C1	C3	0.97400227438
N2	C3	0.044793942774
C1	O4	0.080688015783
N2	O4	1.6856259174
C3	O4	0.011977923085
C1	O5	0.068225924085
N2	O5	1.7002884999
C3	O5	0.039006406417
O4	O5	0.32961165902
C1	H6	0.91991713248
N2	H6	0.058168912905
C3	H6	0.032835496477
O4	H6	0.018881033895
O5	H6	0.012175039134
C1	H7	0.91989047925
N2	H7	0.058304288475
C3	H7	0.032847148344
O4	H7	0.018749781334
O5	H7	0.012171940265
H6	H7	0.032645998222
C1	H8	0.049221285538
N2	H8	0.0096964233592
C3	H8	0.96118221071
O4	H8	0.0024015333056
O5	H8	0.0046853577528
H6	H8	0.0031516403793
H7	H8	0.0031459679463
C1	H9	0.043308902746
N2	H9	0.0038440583987



C3	H9	0.95542936581
O4	H9	0.0013464564049
O5	H9	0.014512180545
H6	H9	0.0098891485575
H7	H9	0.003200263934
H8	H9	0.039260360372
C1	C1	0.043348342047
N2	C1	0.0038670066419
C3	C1	0.95549172934
O4	C1	0.0013466063468
O5	C1	0.01435632481
H6	C1	0.00319142299
H7	C1	0.0098965993324
H8	C1	0.039281826152
H9	C1	0.038552809505

# NITROGENATED BASES

## CYTOSINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.96570426025
N1	N3	0.14105348276
C2	N3	0.75483307606
N1	C4	0.051191999555
C2	C4	0.016105135437
N3	C4	1.0353814647
N1	C5	0.089199680116
C2	C5	0.017404935024
N3	C5	0.14570810564
C4	C5	1.5544128854
N1	C6	1.2294489251
C2	C6	0.026253882909
N3	C6	0.037103487504
C4	C6	0.082021060966
C5	C6	1.057854619
N1	N7	0.21600201178
C2	N7	0.014053512696
N3	N7	0.01384902529
C4	N7	0.021740693426
C5	N7	0.093958326765
C6	N7	0.9522199355
N1	O8	0.21037404552
C2	O8	1.0321558675
N3	O8	0.23985880506
C4	O8	0.013205984575
C5	O8	0.01798216259
C6	O8	0.02090242204
N7	O8	0.0084664434031

N1	H9	0.0089044177596
C2	H9	0.011187152526
N3	H9	0.77170647668
C4	H9	0.015872769084
C5	H9	0.0066344378875
C6	H9	0.0010683389632
N7	H9	0.00057626063779
O8	H9	0.012060749571
N1	N1	0.0031282651858
C2	N1	0.0049821547291
N3	N1	0.066899331395
C4	N1	0.93601655074
C5	N1	0.046916386745
C6	N1	0.0084410914901
N7	N1	0.0019281965416
O8	N1	0.002624316566
H9	N1	0.0028920005931
N1	H11	0.011457142409
C2	H11	0.0011766569162
N3	H11	0.01403745322
C4	H11	0.058242804045
C5	H11	0.97852499027
C6	H11	0.035486564523
N7	H11	0.011367426945
O8	H11	0.0018447854426
H9	H11	0.00097768080379
N1	H11	0.005229350148
N1	H12	0.013755641023
C2	H12	0.00036216882367
N3	H12	0.00054742192557
C4	H12	0.0014637341336
C5	H12	0.0070282099937
C6	H12	0.014919739555
N7	H12	0.7798135515
O8	H12	0.00019042061303
H9	H12	4.2599393995e-05
N1	H12	0.00027529963088
H11	H12	0.00041048564634
N1	H13	0.010565677294
C2	H13	0.0013237435051
N3	H13	0.00044753816563
C4	H13	0.00050900568628
C5	H13	0.0051115891558
C6	H13	0.01497065877
N7	H13	0.81148879345
O8	H13	0.00061209415583
H9	H13	4.6156944876e-05
N1	H13	2.7052510109e-05

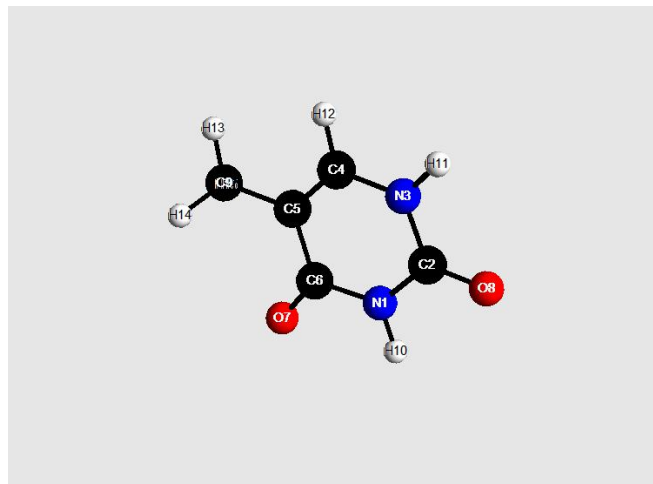
H11	H13	0.003519596587
H12	H13	0.014575042187

### CCSD

Atom A	Atom B	Delocalization index
N1	C2	1.0008027666
N1	N3	0.13316807172
C2	N3	0.78252446198
N1	C4	0.051303595085
C2	C4	0.017391637991
N3	C4	1.0418246306
N1	C5	0.084728963937
C2	C5	0.018188865135
N3	C5	0.14301296949
C4	C5	1.5539933319
N1	C6	1.2704176603
C2	C6	0.030075046264
N3	C6	0.037454686835
C4	C6	0.082255193163
C5	C6	1.0696989147
N1	N7	0.2031737486
C2	N7	0.014738188838
N3	N7	0.013520341837
C4	N7	0.021804688904
C5	N7	0.092018118186
C6	N7	0.97325523383
N1	O8	0.19741763832
C2	O8	1.0622998641
N3	O8	0.22702149784
C4	O8	0.013289462216
C5	O8	0.017528013733
C6	O8	0.021544622108
N7	O8	0.0080804630457
N1	H9	0.0089747403977
C2	H9	0.011984578488
N3	H9	0.77206779643
C4	H9	0.016404396045
C5	H9	0.0066995732704
C6	H9	0.0010906897758
N7	H9	0.00056432476015
O8	H9	0.011746353754
N1	N1	0.0030498862239
C2	N1	0.0051434412447
N3	N1	0.063898686756
C4	N1	0.93571326029
C5	N1	0.046315553778
C6	N1	0.008220567001
N7	N1	0.0018865393001

O8	N1	0.0025496138684
H9	N1	0.0026916340541
N1	H11	0.011284131893
C2	H11	0.0012076224547
N3	H11	0.013705864709
C4	H11	0.057015600871
C5	H11	0.97663035644
C6	H11	0.035579449945
N7	H11	0.011131090806
O8	H11	0.00175500575
H9	H11	0.0010010848151
N1	H11	0.0047854638107
N1	H12	0.013445897774
C2	H12	0.00039198823612
N3	H12	0.00053372036928
C4	H12	0.0014805809072
C5	H12	0.0069868171472
C6	H12	0.015647087473
N7	H12	0.7794100039
O8	H12	0.00017670524268
H9	H12	4.3037186871e-05
N1	H12	0.00026949550081
H11	H12	0.00041334435218
N1	H13	0.010341583601
C2	H13	0.0014370712905
N3	H13	0.00044149097607
C4	H13	0.00050367294407
C5	H13	0.0050470625059
C6	H13	0.015801381899
N7	H13	0.81111585814
O8	H13	0.0006182939659
H9	H13	4.6937807713e-05
N1	H13	2.3769798922e-05
H11	H13	0.0035115222301
H12	H13	0.015006732805

## THYMINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.81726832551
N1	N3	0.14676354882
C2	N3	0.80807014816
N1	C4	0.029716392385
C2	C4	0.015295471505
N3	C4	0.9693822674
N1	C5	0.079867264607
C2	C5	0.012176735781
N3	C5	0.13175093146
C4	C5	1.6245061743
N1	C6	0.81996327283
C2	C6	0.01069156224
N3	C6	0.022037478337
C4	C6	0.084113720798
C5	C6	0.97056816843
N1	O7	0.24707456506
C2	O7	0.010657149609
N3	O7	0.014325107089
C4	O7	0.037519277864
C5	O7	0.11184450639
C6	O7	1.1218955293
N1	O8	0.22920970341
C2	O8	1.0228914244
N3	O8	0.23126519121
C4	O8	0.01250002233
C5	O8	0.013471448012
C6	O8	0.010238494216
O7	O8	0.0073979742788
N1	C9	0.0071757825849
C2	C9	0.0006495919909

N3	C9	0.011573804383
C4	C9	0.058653911232
C5	C9	0.99999951978
C6	C9	0.030869329443
O7	C9	0.027768375267
O8	C9	0.00093038725515
N1	N1	0.75215049707
C2	N1	0.011047418531
N3	N1	0.0073090529336
C4	N1	0.00067826073116
C5	N1	0.0056647289426
C6	N1	0.012146430396
O7	N1	0.01092304463
O8	N1	0.0098086773502
C9	N1	0.00089601318623
N1	H11	0.0076087598667
C2	H11	0.011702902565
N3	H11	0.76776477485
C4	H11	0.014892086314
C5	H11	0.0058338543775
C6	H11	0.00053701265318
O7	H11	0.00051196546302
O8	H11	0.010336468692
C9	H11	0.00084270788054
N1	H11	0.00083992446494
N1	H12	0.0015556604805
C2	H12	0.0047867161994
N3	H12	0.064109263745
C4	H12	0.93555692222
C5	H12	0.047898432187
C6	H12	0.0088117961874
O7	H12	0.0034198116906
O8	H12	0.0021288290439
C9	H12	0.0094041588293
N1	H12	9.9312156868e-05
H11	H12	0.0025809379719
N1	H13	0.0014530667613
C2	H13	0.00011087628715
N3	H13	0.00095878757713
C4	H13	0.01199998379
C5	H13	0.046422390371
C6	H13	0.0072970543307
O7	H13	0.0033003449378
O8	H13	0.00012507975791
C9	H13	0.96113916096
N1	H13	0.00025143767689
H11	H13	3.8035575959e-05
H12	H13	0.0077182778212

N1	H14	0.00065669754279
C2	H14	0.00040329456418
N3	H14	0.0033980143407
C4	H14	0.014926228236
C5	H14	0.045319938675
C6	H14	0.003206759966
O7	H14	0.010556872895
O8	H14	0.00058679620944
C9	H14	0.95103741247
N1	H14	2.5195974925e-05
H11	H14	0.00013789355553
H12	H14	0.00091190199529
H13	H14	0.039773049492
N1	H15	0.00065675274374
C2	H15	0.00040318497224
N3	H15	0.0033974556265
C4	H15	0.014924196759
C5	H15	0.045296004038
C6	H15	0.0032082159782
O7	H15	0.010562606996
O8	H15	0.00058667189579
C9	H15	0.95104485095
N1	H15	2.5200887764e-05
H11	H15	0.00013788282896
H12	H15	0.00091196141991
H13	H15	0.039772394411
H14	H15	0.039353428398

#### CCSD

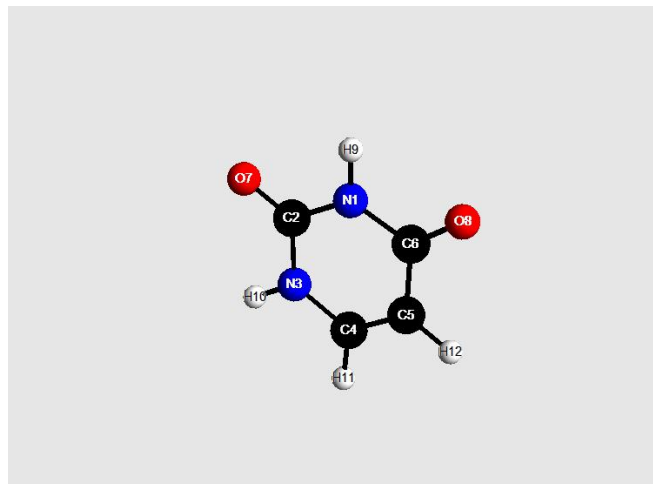
Atom A	Atom B	Delocalization index
N1	C2	0.85147804677
N1	N3	0.13919743775
C2	N3	0.84095597307
N1	C4	0.029877604428
C2	C4	0.016647195952
N3	C4	0.97433508298
N1	C5	0.079040861451
C2	C5	0.013170444771
N3	C5	0.13011991349
C4	C5	1.6179946994
N1	C6	0.83971867131
C2	C6	0.01209910847
N3	C6	0.022205258621
C4	C6	0.084503237086
C5	C6	0.98243008886
N1	O7	0.23332570614
C2	O7	0.011232490942
N3	O7	0.014453411263



C4	07	0.038134759735
C5	07	0.10818567017
C6	07	1.1424031174
N1	08	0.2150795641
C2	08	1.057496694
N3	08	0.21793416134
C4	08	0.012454970977
C5	08	0.013415264533
C6	08	0.010510762803
07	08	0.0070174511713
N1	C9	0.0072503075071
C2	C9	0.00069966439368
N3	C9	0.011364401504
C4	C9	0.058013082732
C5	C9	1.0023602693
C6	C9	0.031681539304
07	C9	0.027988786249
08	C9	0.00092047227944
N1	N1	0.75270920273
C2	N1	0.01200486419
N3	N1	0.0073149984168
C4	N1	0.00068190574099
C5	N1	0.0056869498226
C6	N1	0.012796518606
07	N1	0.010536196029
08	N1	0.0094957916486
C9	N1	0.0009217130553
N1	H11	0.0076274918558
C2	H11	0.012605173775
N3	H11	0.76760861682
C4	H11	0.015312434622
C5	H11	0.0059646027874
C6	H11	0.00053666098237
07	H11	0.0005113423202
08	H11	0.010001899007
C9	H11	0.00086151194566
N1	H11	0.00086543078562
N1	H12	0.001525423061
C2	H12	0.0050490119105
N3	H12	0.061693937439
C4	H12	0.93422718925
C5	H12	0.047307025609
C6	H12	0.0085556707983
07	H12	0.0033257751786
08	H12	0.0020997483151
C9	H12	0.0089243976943
N1	H12	9.4049633244e-05
H11	H12	0.0024318692592

N1	H13	0.0014598129245
C2	H13	0.00011571246895
N3	H13	0.00094910542243
C4	H13	0.012000816008
C5	H13	0.046313264378
C6	H13	0.0073960862479
O7	H13	0.0032928096141
O8	H13	0.00012446423387
C9	H13	0.96085854243
N1	H13	0.0002555841547
H11	H13	3.8509042031e-05
H12	H13	0.0075706328356
N1	H14	0.00065399758087
C2	H14	0.00044431838419
N3	H14	0.0033773341011
C4	H14	0.015089359297
C5	H14	0.045277022451
C6	H14	0.0033502954769
O7	H14	0.010884528387
O8	H14	0.00058766936652
C9	H14	0.94974369761
N1	H14	2.5286362699e-05
H11	H14	0.00014114902045
H12	H14	0.00088312581777
H13	H14	0.038953607984
N1	H15	0.00065404707511
C2	H15	0.00044430319476
N3	H15	0.0033771038372
C4	H15	0.015088180052
C5	H15	0.045258467391
C6	H15	0.0033544938354
O7	H15	0.010886592403
O8	H15	0.00058760451919
C9	H15	0.94976864323
N1	H15	2.5288414896e-05
H11	H15	0.00014116598081
H12	H15	0.00088311834856
H13	H15	0.03895346755
H14	H15	0.038648927442

## URACIL

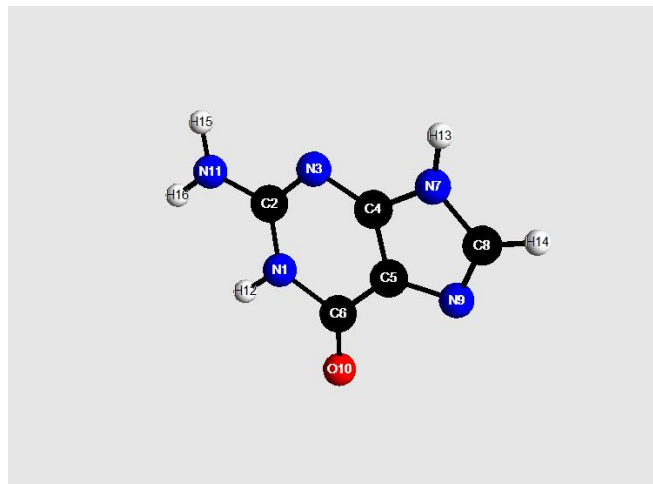


## HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.82638499652
N1	N3	0.14307188368
C2	N3	0.80181342825
N1	C4	0.029149441253
C2	C4	0.015096258328
N3	C4	0.98044089154
N1	C5	0.08333015319
C2	C5	0.012470282647
N3	C5	0.13855301319
C4	C5	1.6355187097
N1	C6	0.81427380007
C2	C6	0.010843308887
N3	C6	0.021533657291
C4	C6	0.0811471973
C5	C6	0.98558047976
N1	O7	0.2300873633
C2	O7	1.028187038
N3	O7	0.22965059431
C4	O7	0.01253768938
C5	O7	0.014256268051
C6	O7	0.010388524562
N1	O8	0.24585111164
C2	O8	0.010872807347
N3	O8	0.014951482481
C4	O8	0.039773638493
C5	O8	0.12023381134
C6	O8	1.1271486889
O7	O8	0.0075635981198
N1	H9	0.75123563532
C2	H9	0.011202051924

N3	H9	0.0072825858194
C4	H9	0.0006950376416
C5	H9	0.0057376039172
C6	H9	0.012063204325
O7	H9	0.0097956855564
O8	H9	0.010782275281
N1	N1	0.0074048409013
C2	N1	0.011638180288
N3	N1	0.76465501838
C4	N1	0.015008488946
C5	N1	0.0060267402243
C6	N1	0.00052923084858
O7	N1	0.01027412717
O8	N1	0.00052788869036
H9	N1	0.00080908031598
N1	H11	0.0015403517262
C2	H11	0.0048649979986
N3	H11	0.064063884195
C4	H11	0.93786048607
C5	H11	0.048101585244
C6	H11	0.0086812139052
O7	H11	0.002206995556
O8	H11	0.0032995076696
H9	H11	0.00010048706987
N1	H11	0.002560697322
N1	H12	0.008270463479
C2	H12	0.00064442476531
N3	H12	0.013273850276
C4	H12	0.058597298162
C5	H12	0.96416846639
C6	H12	0.031027434762
O7	H12	0.0011635267109
O8	H12	0.012232515532
H9	H12	0.0010466567143
N1	H12	0.00096234397421
H11	H12	0.0055362727811

## GUANINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	0.90697433378
N1	N3	0.1646387894
C2	N3	1.2073730929
N1	C4	0.035921323767
C2	C4	0.029073975296
N3	C4	1.0736080332
N1	C5	0.092774740967
C2	C5	0.027492985425
N3	C5	0.083422818517
C4	C5	1.2830156518
N1	C6	0.77473826942
C2	C6	0.01303353284
N3	C6	0.021312918469
C4	C6	0.072647446588
C5	C6	1.0266749128
N1	N7	0.007659020322
C2	N7	0.012542206478
N3	N7	0.12417580462
C4	N7	0.96103920745
C5	N7	0.13499852825
C6	N7	0.014771998414
N1	C8	0.0041663650212
C2	C8	0.0060441711066
N3	C8	0.011420376855
C4	C8	0.056739688864
C5	C8	0.064286931835
C6	C8	0.016230071914
N7	C8	0.91963182752
N1	N9	0.012323623676
C2	N9	0.0052159980864

N3	N9	0.019666138078
C4	N9	0.11064527635
C5	N9	1.1059730104
C6	N9	0.051640599495
N7	N9	0.24119898609
C8	N9	1.3784626556
N1	N1	0.23747130099
C2	N1	0.01058478749
N3	N1	0.017507104351
C4	N1	0.029798086632
C5	N1	0.11142210733
C6	N1	1.1176238489
N7	N1	0.0079059443806
C8	N1	0.0078627799851
N9	N1	0.022216022958
N1	N11	0.16354321858
C2	N11	0.91071425229
N3	N11	0.19066660953
C4	N11	0.01223781266
C5	N11	0.011979744972
C6	N11	0.0067890394639
N7	N11	0.0039421073162
C8	N11	0.0029897152663
N9	N11	0.0025427949673
N1	N11	0.0040650951373
N1	H12	0.77866070754
C2	H12	0.013087091912
N3	H12	0.0099771718276
C4	H12	0.001064725914
C5	H12	0.0053004385329
C6	H12	0.012528548581
N7	H12	0.00029747370673
C8	H12	0.00014709182686
N9	H12	0.0011052877706
N1	H12	0.013534559252
N11	H12	0.0079899221291
N1	H13	0.00020559595721
C2	H13	0.00017431003286
N3	H13	0.0045980253781
C4	H13	0.014583498274
C5	H13	0.0065264402514
C6	H13	0.00094814919026
N7	H13	0.77119564297
C8	H13	0.013057576819
N9	H13	0.011127848746
N1	H13	0.0005296889573
N11	H13	6.5400970058e-05
H12	H13	1.6466615466e-05

N1	H14	0.0006128919779
C2	H14	0.00066873394893
N3	H14	0.0017984426385
C4	H14	0.0079290199367
C5	H14	0.012233454558
C6	H14	0.0018498858277
N7	H14	0.061024887171
C8	H14	0.91810854121
N9	H14	0.073249738375
N1	H14	0.00078468947233
N11	H14	0.00032512508797
H12	H14	5.1648390503e-05
H13	H14	0.00078266385824
N1	H15	0.008766879175
C2	H15	0.013264432679
N3	H15	0.011141448691
C4	H15	0.00038634893591
C5	H15	0.00037925198467
C6	H15	0.00078307756887
N7	H15	9.4789589688e-05
C8	H15	6.3066384751e-05
N9	H15	0.00010652837171
N1	H15	0.00055215534299
N11	H15	0.77741339054
H12	H15	0.0003076137346
H13	H15	5.6882041664e-06
H14	H15	9.4984135771e-06
N1	H16	0.0069183077441
C2	H16	0.014532313897
N3	H16	0.0098493941975
C4	H16	0.0013262635381
C5	H16	0.00046884152606
C6	H16	0.00025058091912
N7	H16	0.00028259558953
C8	H16	0.00012163574016
N9	H16	0.00013333796775
N1	H16	0.00010036954016
N11	H16	0.80607362335
H12	H16	0.0021371299947
H13	H16	4.7401015155e-06
H14	H16	1.9041056236e-05
H15	H16	0.014052087881

#### CCSD

Atom A	Atom B	Delocalization index
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N1	N3	0.15213332946
C2	N3	1.2598648098

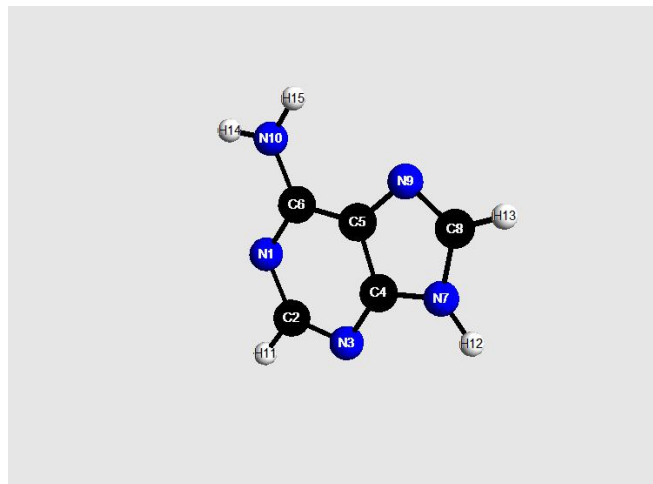
N1	C4	0.036163236315
C2	C4	0.032989277721
N3	C4	1.0935379388
N1	C5	0.091613973823
C2	C5	0.028886228754
N3	C5	0.080186476828
C4	C5	1.2836844454
N1	C6	0.79344962766
C2	C6	0.014527195291
N3	C6	0.021288568019
C4	C6	0.073447481719
C5	C6	1.0347682506
N1	N7	0.0074093421643
C2	N7	0.013343304502
N3	N7	0.11759048745
C4	N7	0.97196371453
C5	N7	0.13178595061
C6	N7	0.014628107633
N1	C8	0.0043309248227
C2	C8	0.0066992112912
N3	C8	0.011421247405
C4	C8	0.060204279795
C5	C8	0.067810629981
C6	C8	0.017450644302
N7	C8	0.94060351862
N1	N9	0.012285390269
C2	N9	0.0053225105866
N3	N9	0.018826177759
C4	N9	0.10701265402
C5	N9	1.1212119012
C6	N9	0.05090521139
N7	N9	0.22729164797
C8	N9	1.4184581516
N1	N1	0.22429430913
C2	N1	0.011074796005
N3	N1	0.017196433187
C4	N1	0.030045730136
C5	N1	0.10839813523
C6	N1	1.1387664545
N7	N1	0.0076881916787
C8	N1	0.0081789330971
N9	N1	0.021771166816
N1	N11	0.15380394856
C2	N11	0.9459022508
N3	N11	0.1774486635
C4	N11	0.012410891643
C5	N11	0.0116998046
C6	N11	0.0069773647291



N7	N11	0.0038967907531
C8	N11	0.0030872013841
N9	N11	0.00239150519
N1	N11	0.003871677289
N1	H12	0.77847892963
C2	H12	0.014114463884
N3	H12	0.0098482624082
C4	H12	0.0010953633039
C5	H12	0.0053596857971
C6	H12	0.013161265844
N7	H12	0.00028495725011
C8	H12	0.00016232553134
N9	H12	0.0011264085864
N1	H12	0.013152943543
N11	H12	0.0077318263607
N1	H13	0.00020047623692
C2	H13	0.0001915953619
N3	H13	0.0044374227811
C4	H13	0.01508268124
C5	H13	0.0065540407965
C6	H13	0.0009438119371
N7	H13	0.76934852732
C8	H13	0.013680549089
N9	H13	0.011094650764
N1	H13	0.00052412050278
N11	H13	6.1024657517e-05
H12	H13	1.5971791552e-05
N1	H14	0.00060561806346
C2	H14	0.00070349365611
N3	H14	0.0017366506101
C4	H14	0.0080443002808
C5	H14	0.011841195472
C6	H14	0.0018965867402
N7	H14	0.059288895575
C8	H14	0.92154307599
N9	H14	0.067513126596
N1	H14	0.00077286912941
N11	H14	0.00031969878457
H12	H14	5.3428425232e-05
H13	H14	0.00073402488092
N1	H15	0.0086678446539
C2	H15	0.014328125668
N3	H15	0.010707888923
C4	H15	0.00039971027272
C5	H15	0.00037524855441
C6	H15	0.00083425004801
N7	H15	8.7555791941e-05
C8	H15	6.5025997526e-05

N9	H15	0.0001030401777
N1	H15	0.00055368523047
N11	H15	0.77697032062
H12	H15	0.00030408402674
H13	H15	5.4675026953e-06
H14	H15	8.9308495213e-06
N1	H16	0.0066737094897
C2	H16	0.015689620729
N3	H16	0.0095780780004
C4	H16	0.0013787884174
C5	H16	0.0004557578224
C6	H16	0.00025280849849
N7	H16	0.00029136350387
C8	H16	0.00012607576503
N9	H16	0.00012749899089
N1	H16	9.6437058249e-05
N11	H16	0.80415301528
H12	H16	0.0021260540829
H13	H16	4.2061456941e-06
H14	H16	1.9567434392e-05
H15	H16	0.014460537174

## ADENINE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
N1	C2	1.1379853734
N1	N3	0.19076364781
C2	N3	1.1943377706
N1	C4	0.058365690822
C2	C4	0.032445766384
N3	C4	1.1639343466
N1	C5	0.098577174431
C2	C5	0.052889187621
N3	C5	0.087867782405
C4	C5	1.2166636034
N1	C6	1.175759933
C2	C6	0.028121387827
N3	C6	0.058017529019
C4	C6	0.073704756442
C5	C6	1.1419967467
N1	N7	0.015117917785
C2	N7	0.013641216657
N3	N7	0.12808377588
C4	N7	0.93170747848
C5	N7	0.12584685325
C6	N7	0.013521462382
N1	C8	0.0071443023968
C2	C8	0.01133779833
N3	C8	0.011493346691
C4	C8	0.046832051652
C5	C8	0.057251824238
C6	C8	0.022606490797
N7	C8	0.93625528555
N1	N9	0.018252886744
C2	N9	0.0089039847391

N3	N9	0.019176718351
C4	N9	0.099725579208
C5	N9	1.0914405986
C6	N9	0.058345846851
N7	N9	0.23992376092
C8	N9	1.3615192497
N1	N1	0.18071454295
C2	N1	0.011629653584
N3	N1	0.024056597875
C4	N1	0.017492628571
C5	N1	0.094452478615
C6	N1	0.97025541782
N7	N1	0.0043526461988
C8	N1	0.0063236694159
N9	N1	0.022021991497
N1	H11	0.074339648877
C2	H11	0.90170654189
N3	H11	0.077961240773
C4	H11	0.0085237228208
C5	H11	0.0038737905401
C6	H11	0.0079082421586
N7	H11	0.001630943536
C8	H11	0.0010201851187
N9	H11	0.00082016244261
N1	H11	0.0011991989316
N1	H12	0.00039679654225
C2	H12	0.00016481739846
N3	H12	0.0043429315522
C4	H12	0.014092929589
C5	H12	0.0065033260681
C6	H12	0.00087252040456
N7	H12	0.7672065273
C8	H12	0.013301380035
N9	H12	0.010710365914
N1	H12	0.00032029510057
H11	H12	2.6089072554e-05
N1	H13	0.00092245881293
C2	H13	0.0011246710526
N3	H13	0.0017104609993
C4	H13	0.0071531728865
C5	H13	0.011526115751
C6	H13	0.0023495297011
N7	H13	0.060996863575
C8	H13	0.91531866057
N9	H13	0.072337698352
N1	H13	0.00056181444392
H11	H13	0.0001168134284
H12	H13	0.0008321180781

N1	H14	0.012229814572
C2	H14	0.00030677095712
N3	H14	0.00078310343563
C4	H14	0.0011746854261
C5	H14	0.0069317361336
C6	H14	0.01542133648
N7	H14	0.00034121348259
C8	H14	0.00018044459337
N9	H14	0.00077621037903
N1	H14	0.78865583694
H11	H14	9.2369133932e-05
H12	H14	5.6099091034e-05
H13	H14	1.8391980655e-05
N1	H15	0.0090892168265
C2	H15	0.0010264547822
N3	H15	0.00071150835793
C4	H15	0.00030566192893
C5	H15	0.0025560720408
C6	H15	0.014315087524
N7	H15	0.00028447780028
C8	H15	0.00055039401127
N9	H15	0.0090212905272
N1	H15	0.78842646002
H11	H15	0.00017921147501
H12	H15	3.0049399103e-05
H13	H15	2.5372103485e-05
H14	H15	0.014337697821

#### CCSD

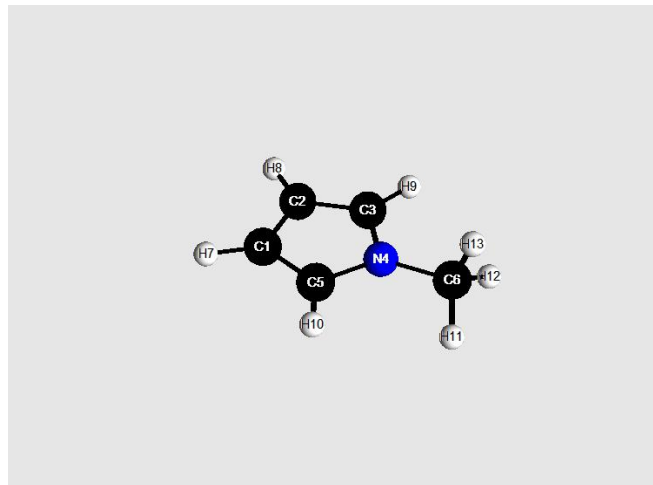
Atom A	Atom B	Delocalization index
N1	C2	1.1801472283
N1	N3	0.1738188149
C2	N3	1.2336017002
N1	C4	0.057839658096
C2	C4	0.036290316049
N3	C4	1.1903970304
N1	C5	0.093672510905
C2	C5	0.054627531301
N3	C5	0.083545474638
C4	C5	1.2197612801
N1	C6	1.2034404005
C2	C6	0.031698090959
N3	C6	0.057810922826
C4	C6	0.074579396434
C5	C6	1.1485360612
N1	N7	0.014430094801
C2	N7	0.014352795144
N3	N7	0.12081387736

C4	N7	0.94265184725
C5	N7	0.12314685744
C6	N7	0.013358772587
N1	C8	0.0071471975047
C2	C8	0.012365015486
N3	C8	0.01145140856
C4	C8	0.050120441127
C5	C8	0.061168430334
C6	C8	0.02414020849
N7	C8	0.95897309769
N1	N9	0.017838550857
C2	N9	0.0088312345163
N3	N9	0.018304727463
C4	N9	0.096987948667
C5	N9	1.1053506609
C6	N9	0.056997296744
N7	N9	0.22567782934
C8	N9	1.4052299445
N1	N1	0.17029396299
C2	N1	0.012286086504
N3	N1	0.023287809847
C4	N1	0.01760970054
C5	N1	0.092855271968
C6	N1	0.98865712271
N7	N1	0.0042582764716
C8	N1	0.006591323901
N9	N1	0.021976214755
N1	H11	0.069321624359
C2	H11	0.90717407932
N3	H11	0.072877714909
C4	H11	0.0086754194076
C5	H11	0.0037599931223
C6	H11	0.0080716465227
N7	H11	0.0016737714401
C8	H11	0.0010558307144
N9	H11	0.00075992772724
N1	H11	0.0012110704152
N1	H12	0.0003787451225
C2	H12	0.00017936928219
N3	H12	0.0041735577974
C4	H12	0.014602562103
C5	H12	0.0065681157873
C6	H12	0.00087552052399
N7	H12	0.76576489059
C8	H12	0.013992483751
N9	H12	0.010660329078
N1	H12	0.00032262251892
H11	H12	2.1849938953e-05

N1	H13	0.00088643201098
C2	H13	0.0011681559351
N3	H13	0.0016453923488
C4	H13	0.007273884679
C5	H13	0.011194932571
C6	H13	0.0023969126439
N7	H13	0.059112133033
C8	H13	0.91903384285
N9	H13	0.06649960304
N1	H13	0.00055414454961
H11	H13	0.0001189016423
H12	H13	0.00077588927288
N1	H14	0.011741713944
C2	H14	0.00032862559283
N3	H14	0.00075918796124
C4	H14	0.0012019898789
C5	H14	0.0069677118472
C6	H14	0.016126859037
N7	H14	0.00034291198682
C8	H14	0.00018614069642
N9	H14	0.00079074496442
N1	H14	0.78880754371
H11	H14	7.8860750212e-05
H12	H14	5.8397422145e-05
H13	H14	1.7881814816e-05
N1	H15	0.008902672131
C2	H15	0.0011191736131
N3	H15	0.00068433029639
C4	H15	0.00030855115646
C5	H15	0.0025140008022
C6	H15	0.015003486343
N7	H15	0.00028959266634
C8	H15	0.00063578198341
N9	H15	0.0094188189331
N1	H15	0.78702635322
H11	H15	0.00019210998813
H12	H15	3.1546967536e-05
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# PYRROLES

## N-METHYLPYRROLE



### HARTREE-FOCK

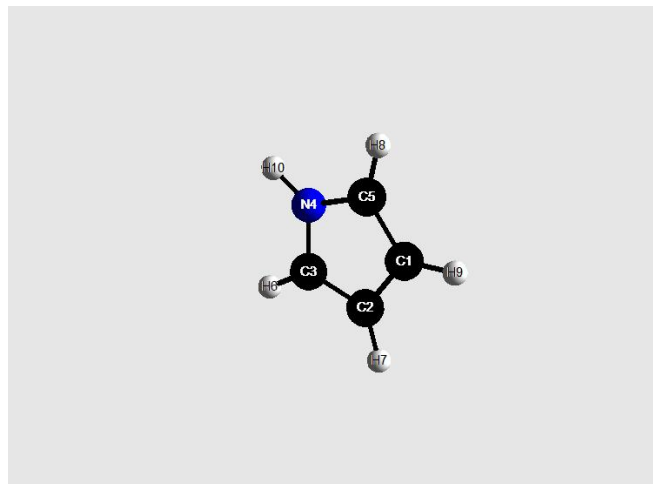
Atom A	Atom B	Delocalization index
C1	C2	1.2526626552
C1	C3	0.090260487229
C2	C3	1.486056877
C1	N4	0.1684631557
C2	N4	0.16848964072
C3	N4	1.0416219406
C1	C5	1.4860342269
C2	C5	0.090284017277
C3	C5	0.12703652035
N4	C5	1.0416337624
C1	C6	0.008320421526
C2	C6	0.0083239175457
C3	C6	0.02307552318
N4	C6	0.88212109627
C5	C6	0.023101200875
C1	H7	0.98938486742
C2	H7	0.040546449583
C3	H7	0.0089887288998
N4	H7	0.015100105878
C5	H7	0.054699617045
C6	H7	0.0013452228456
C1	H8	0.040548485464
C2	H8	0.98934043868
C3	H8	0.054705544046
N4	H8	0.015099928708
C5	H8	0.0089880906371
C6	H8	0.0013454495405
H7	H8	0.0025536729449



C1	H9	0.010185239058
C2	H9	0.047649156104
C3	H9	0.95792048623
N4	H9	0.064193442654
C5	H9	0.014211862047
C6	H9	0.0059957015185
H7	H9	0.0015501582953
H8	H9	0.0029397101346
C1	C1	0.047646088466
C2	C1	0.010187140976
C3	C1	0.014213303035
N4	C1	0.064186201257
C5	C1	0.95790528359
C6	C1	0.0060046365658
H7	C1	0.0029397225708
H8	C1	0.0015500202429
H9	C1	0.0021524374043
C1	H11	0.0018263325662
C2	H11	0.0021447968387
C3	H11	0.0066010123902
N4	H11	0.066065023716
C5	H11	0.0078686440995
C6	H11	0.93567516645
H7	H11	0.00013015203551
H8	H11	0.0004158154417
H9	H11	0.0006261843127
C1	H11	0.0061745489819
C1	H12	0.0021478117229
C2	H12	0.0018307656449
C3	H12	0.0078626113301
N4	H12	0.066085783217
C5	H12	0.0065998864683
C6	H12	0.93562213058
H7	H12	0.00041580900087
H8	H12	0.00013044090584
H9	H12	0.0061667449863
C1	H12	0.00062518393877
H11	H12	0.038022681335
C1	H13	0.0041327462434
C2	H13	0.004130898087
C3	H13	0.0053238139563
N4	H13	0.068170072054
C5	H13	0.0053232242064
C6	H13	0.93624276401
H7	H13	0.00033257207969
H8	H13	0.00033224963888
H9	H13	0.00038841225255
C1	H13	0.00038666742088

H11	H13	0.039242261308
H12	H13	0.039244854601

## PYRROLE



## HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.2396362895
C1	C3	0.08993376798
C2	C3	1.4996496724
C1	N4	0.1750379207
C2	N4	0.17504848043
C3	N4	1.0358904209
C1	C5	1.4996829088
C2	C5	0.089915816854
C3	C5	0.12787087747
N4	C5	1.0358761598
C1	H6	0.0103475099
C2	H6	0.047125717418
C3	H6	0.95983618309
N4	H6	0.065530629814
C5	H6	0.013960029187
C1	H7	0.039751527596
C2	H7	0.98740272991
C3	H7	0.054956836606
N4	H7	0.015586570729
C5	H7	0.0087924531708
H6	H7	0.0028950012207
C1	H8	0.047122972534
C2	H8	0.010347962952
C3	H8	0.013959974305
N4	H8	0.065525944632
C5	H8	0.95982875625
H6	H8	0.0019789485316
H7	H8	0.0015850045051
C1	H9	0.98744207408
C2	H9	0.039744556587

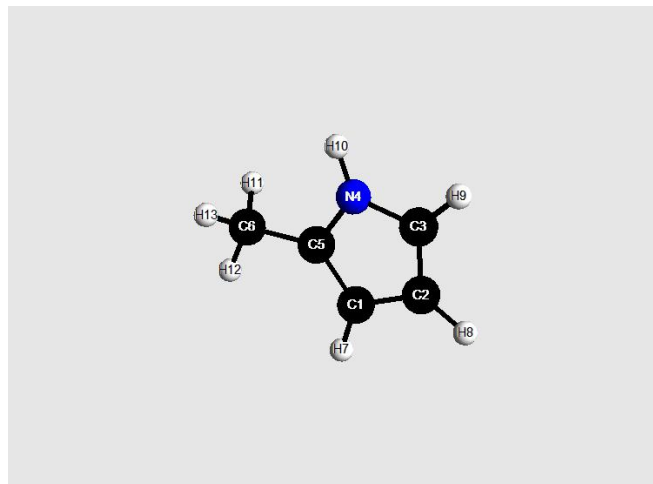
C3	H9	0.0087949576813
N4	H9	0.015588310782
C5	H9	0.054952702722
H6	H9	0.0015849127083
H7	H9	0.0024707266325
H8	H9	0.0028945210166
C1	C1	0.0081250253011
C2	C1	0.0081261548093
C3	C1	0.016137830669
N4	C1	0.79637127608
C5	C1	0.016134476833
H6	C1	0.0014727075915
H7	C1	0.0014491801244
H8	C1	0.0014731149939
H9	C1	0.0014490044068

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.068100778
C1	C3	0.066811037413
C2	C3	1.2227642842
C1	N4	0.11810992764
C2	N4	0.1181171659
C3	N4	0.94995918152
C1	C5	1.2227647939
C2	C5	0.066803893135
C3	C5	0.091000302251
N4	C5	0.94997406981
C1	H6	0.0079391347577
C2	H6	0.033686168393
C3	H6	0.83627253538
N4	H6	0.046069548793
C5	H6	0.010630548522
C1	H7	0.030432122148
C2	H7	0.85354196092
C3	H7	0.038874716103
N4	H7	0.011042289353
C5	H7	0.0069114552466
H6	H7	0.0021921048382
C1	H8	0.03367542456
C2	H8	0.0079401541688
C3	H8	0.010630317356
N4	H8	0.046071067372
C5	H8	0.8363119411
H6	H8	0.0017533433658
H7	H8	0.0014728387529
C1	H9	0.85352023155
C2	H9	0.030431870105

C3	H9	0.0069123160444
N4	H9	0.011042365209
C5	H9	0.03887714872
H6	H9	0.0014728374612
H7	H9	0.0021390649936
H8	H9	0.0021921580361
C1	C1	0.0069896501218
C2	C1	0.006990039393
C3	C1	0.01518248827
N4	C1	0.71761710522
C5	C1	0.015183014127
H6	C1	0.0014031165561
H7	C1	0.0014484671002
H8	C1	0.0014031466703
H9	C1	0.0014484578093

## 2-METHYLPYRROLE



### HARTREE-FOCK

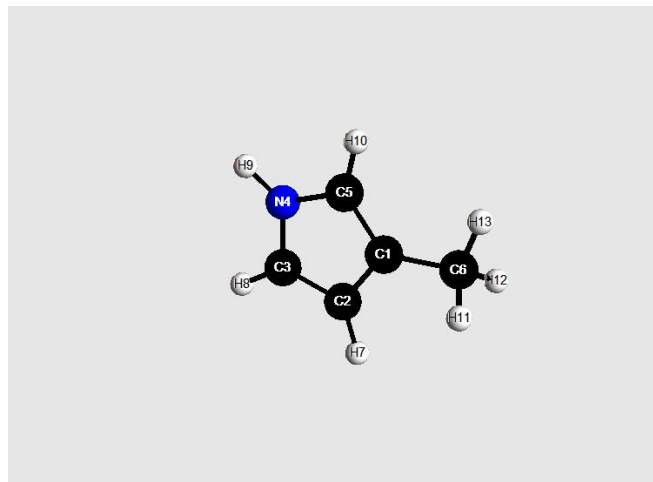
Atom A	Atom B	Delocalization index
C1	C2	1.2260021454
C1	C3	0.090866148348
C2	C3	1.5191492904
C1	N4	0.16900925851
C2	N4	0.17293292559
C3	N4	1.0267150984
C1	C5	1.4831500236
C2	C5	0.084755776985
C3	C5	0.1172459277
N4	C5	1.015820035
C1	C6	0.046500316205
C2	C6	0.0085956526448
C3	C6	0.011029481728
N4	C6	0.070991348028
C5	C6	0.99341827691
C1	H7	0.98841209564
C2	H7	0.039765633585
C3	H7	0.0089067494311
N4	H7	0.015328451747
C5	H7	0.055070147089
C6	H7	0.0050061251704
C1	H8	0.039366800019
C2	H8	0.98896120277
C3	H8	0.056296476956
N4	H8	0.015695816326
C5	H8	0.0084392100659
C6	H8	0.0013050236596
H7	H8	0.0024412487935
C1	H9	0.010709495905
C2	H9	0.048513150688

C3	H9	0.96306492871
N4	H9	0.064435306167
C5	H9	0.013224649205
C6	H9	0.0016504555069
H7	H9	0.0016029397653
H8	H9	0.0030448109033
C1	C1	0.0084506880685
C2	C1	0.0080321186078
C3	C1	0.016444996997
N4	C1	0.80307740841
C5	C1	0.016474118386
C6	C1	0.0030766040614
H7	C1	0.0015671974744
H8	C1	0.0014269871524
H9	C1	0.0014638671729
C1	H11	0.012783378288
C2	H11	0.0022648315084
C3	H11	0.0040291901982
N4	H11	0.0094912864479
C5	H11	0.044718782109
C6	H11	0.95866373719
H7	H11	0.00069158462463
H8	H11	0.00027420905905
H9	H11	0.00034516042715
C1	H11	0.00077661937362
C1	H12	0.0091414783593
C2	H12	0.00085836132054
C3	H12	0.0013466827781
N4	H12	0.010513206821
C5	H12	0.044028560136
C6	H12	0.96001892473
H7	H12	0.0040432504435
H8	H12	8.4879941776e-05
H9	H12	0.00040302639553
C1	H12	0.00039455321628
H11	H12	0.041019476622
C1	H13	0.012836644171
C2	H13	0.0022696516231
C3	H13	0.0040700491382
N4	H13	0.0094404491652
C5	H13	0.044742386978
C6	H13	0.95862610724
H7	H13	0.0006929830369
H8	H13	0.00027224293813
H9	H13	0.00034854919077
C1	H13	0.00075218138066
H11	H13	0.042499719461
H12	H13	0.041008378478





### 3-METHYLPYRROLE



### HARTREE-FOCK

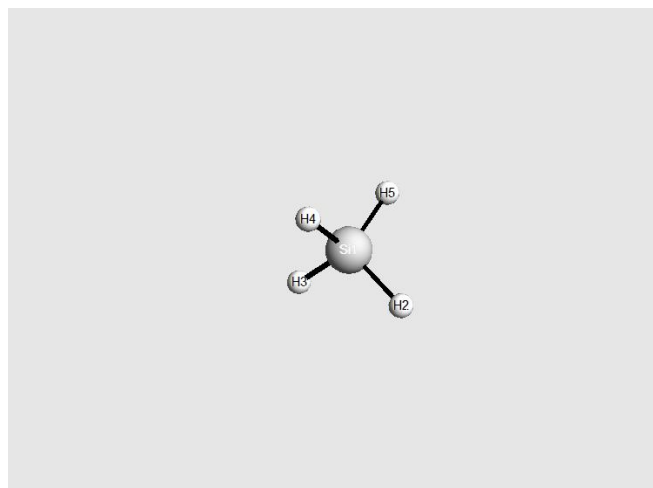
Atom A	Atom B	Delocalization index
C1	C2	1.2179084574
C1	C3	0.086057189123
C2	C3	1.4982170772
C1	N4	0.1657577764
C2	N4	0.1764138871
C3	N4	1.0463133443
C1	C5	1.4872592418
C2	C5	0.088218807606
C3	C5	0.12626285703
N4	C5	1.0288516114
C1	C6	1.0136340699
C2	C6	0.040838749981
C3	C6	0.0083102207067
N4	C6	0.012917960856
C5	C6	0.053710960651
C1	H7	0.039283230199
C2	H7	0.98831827085
C3	H7	0.055916379883
N4	H7	0.015653408884
C5	H7	0.0086705207866
C6	H7	0.0042624268891
C1	H8	0.010014736583
C2	H8	0.047376665175
C3	H8	0.96033377522
N4	H8	0.065887306656
C5	H8	0.014199599745
C6	H8	0.0013565326588
H7	H8	0.0029881437565
C1	H9	0.0078688485908
C2	H9	0.008358297216

C3	H9	0.016533334604
N4	H9	0.79988223513
C5	H9	0.016174730465
C6	H9	0.001246541821
H7	H9	0.0014781435272
H8	H9	0.0015355980336
C1	C1	0.047705780242
C2	C1	0.010126216513
C3	C1	0.013950711872
N4	C1	0.064801971641
C5	C1	0.96125245415
C6	C1	0.004812009493
H7	C1	0.0017028810662
H8	C1	0.001994244384
H9	C1	0.0014360767879
C1	H11	0.045698754137
C2	H11	0.0069289386057
C3	H11	0.0012187551189
N4	H11	0.0041202178881
C5	H11	0.013178436842
C6	H11	0.95996284751
H7	H11	0.0010882575339
H8	H11	0.00011909765963
H9	H11	0.00021408335735
C1	H11	0.00066575609892
C1	H12	0.045681314756
C2	H12	0.0069175670194
C3	H12	0.0012129298743
N4	H12	0.004084354847
C5	H12	0.013167275095
C6	H12	0.96001108601
H7	H12	0.0011024387942
H8	H12	0.00011847748121
H9	H12	0.00022819200922
C1	H12	0.00066655593088
H11	H12	0.043245925763
C1	H13	0.044775196374
C2	H13	0.0085934270005
C3	H13	0.001734360676
N4	H13	0.0010602892595
C5	H13	0.010655852387
C6	H13	0.96305235365
H7	H13	0.00045881801125
H8	H13	0.00040262816929
H9	H13	3.8749029372e-05
C1	H13	0.0040371757087
H11	H13	0.042822781592
H12	H13	0.042822692505



## SILICON COMPOUNDS

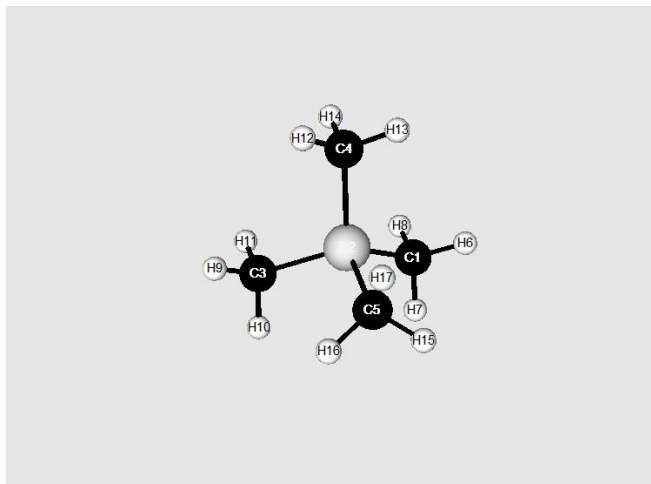
### SILANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
Si1	H2	0.4767373251
Si1	H3	0.47673054735
H2	H3	0.10754879703
Si1	H4	0.4767551587
H2	H4	0.10754511968
H3	H4	0.10754517765
Si1	H5	0.47674479457
H2	H5	0.10754496961
H3	H5	0.10754522454
H4	H5	0.10754791368

## TETRAMETHYLSILANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	Si2	0.40904696619
C1	C3	0.098984322697
Si2	C3	0.40906700472
C1	C4	0.098997924208
Si2	C4	0.40815026514
C3	C4	0.099001569567
C1	C5	0.096184734935
Si2	C5	0.40851866766
C3	C5	0.096195687354
C4	C5	0.096188000427
C1	H6	1.0107976916
Si2	H6	0.01264501215
C3	H6	0.0088334202563
C4	H6	0.0046381254297
C5	H6	0.0044449213345
C1	H7	1.0107186323
Si2	H7	0.012586731505
C3	H7	0.0046362983889
C4	H7	0.0088330772994
C5	H7	0.0044461764195
H6	H7	0.045133182235
C1	H8	1.010777092
Si2	H8	0.012463125799
C3	H8	0.0045939139009
C4	H8	0.0045923551909
C5	H8	0.0084884016981
H6	H8	0.044941419682
H7	H8	0.044941507137
C1	H9	0.0088307175361
Si2	H9	0.012637021475

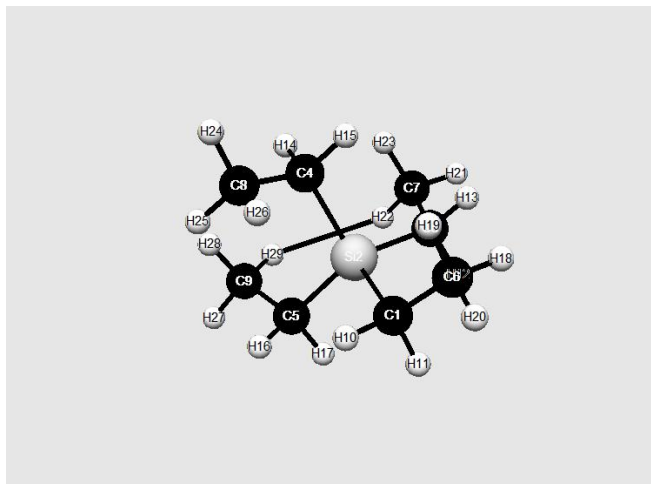
C3	H9	1.0108243083
C4	H9	0.0046339217623
C5	H9	0.0044454062231
H6	H9	0.0014055506801
H7	H9	0.0003924543513
H8	H9	0.00039440844897
C1	C1	0.004632046959
Si2	C1	0.012592488337
C3	C1	1.0107812917
C4	C1	0.0088312729714
C5	C1	0.0044468176626
H6	C1	0.00039253950803
H7	C1	0.0016763367878
H8	C1	0.00022484251234
H9	C1	0.045133111169
C1	H11	0.0045905049399
Si2	H11	0.012468571456
C3	H11	1.0107989846
C4	H11	0.0045918033573
C5	H11	0.0084893399653
H6	H11	0.00039434861408
H7	H11	0.00022480531083
H8	H11	0.0016912065548
H9	H11	0.044941572005
C1	H11	0.044940994888
C1	H12	0.0088327383246
Si2	H12	0.012514722701
C3	H12	0.0046405299052
C4	H12	1.0107088465
C5	H12	0.0044489033155
H6	H12	0.00039259598771
H7	H12	0.0014056191382
H8	H12	0.00039435679233
H9	H12	0.0016769319696
C1	H12	0.00039263772826
H11	H12	0.00022487203357
C1	H13	0.0046343656906
Si2	H13	0.012533073123
C3	H13	0.0088365223767
C4	H13	1.0107257244
C5	H13	0.004446600711
H6	H13	0.0016765966595
H7	H13	0.00039247347384
H8	H13	0.00022482518051
H9	H13	0.00039249667688
C1	H13	0.0014056065058
H11	H13	0.000394459531
H12	H13	0.045132955474

C1	H14	0.0045968111341
Si2	H14	0.012392541415
C3	H14	0.0045978970442
C4	H14	1.0106956982
C5	H14	0.0084935449106
H6	H14	0.00022489089311
H7	H14	0.00039452563209
H8	H14	0.0016918156209
H9	H14	0.00022484580325
C1	H14	0.0003943466956
H11	H14	0.0016914613663
H12	H14	0.044941355807
H13	H14	0.044941578561
C1	H15	0.0099324859028
Si2	H15	0.01209226984
C3	H15	0.004737245324
C4	H15	0.0047249096127
C5	H15	1.0104310608
H6	H15	0.00190683433
H7	H15	0.0019030747627
H8	H15	0.0011490888579
H9	H15	0.00040001533129
C1	H15	0.00011967932223
H11	H15	0.0006983250968
H12	H15	0.00039961859386
H13	H15	0.00011959511459
H14	H15	0.00069664081407
C1	H16	0.0047284679451
Si2	H16	0.012087402615
C3	H16	0.0099381330495
C4	H16	0.0047332745845
C5	H16	1.0104351649
H6	H16	0.00039969525836
H7	H16	0.00011958171183
H8	H16	0.00069665850846
H9	H16	0.0019029865886
C1	H16	0.0019069418088
H11	H16	0.0011490903256
H12	H16	0.00011964703871
H13	H16	0.00040001794363
H14	H16	0.00069830097204
H15	H16	0.045010106337
C1	H17	0.0047355630037
Si2	H17	0.012062643701
C3	H17	0.004727256757
C4	H17	0.0099225665342
C5	H17	1.0105474296
H6	H17	0.00011968746931

H7	H17	0.00039999216185
H8	H17	0.00069831754117
H9	H17	0.00011958075436
C1	H17	0.00039970536184
H11	H17	0.00069665521976
H12	H17	0.0019061368722
H13	H17	0.0019031863
H14	H17	0.0011490049208
H15	H17	0.045009752969
H16	H17	0.045009955807



## TETRAETHYLSILANE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	Si2	0.40565840878
C1	C3	0.093930048731
Si2	C3	0.409559486
C1	C4	0.090103467082
Si2	C4	0.40951845222
C3	C4	0.093360722226
C1	C5	0.095870375847
Si2	C5	0.40944241408
C3	C5	0.089778232759
C4	C5	0.090560832227
C1	C6	1.0181290515
Si2	C6	0.011385138464
C3	C6	0.0059020877916
C4	C6	0.0054439534307
C5	C6	0.0074661944522
C1	C7	0.0075915008498
Si2	C7	0.011322422824
C3	C7	1.0182239761
C4	C7	0.0051011042901
C5	C7	0.003720485647
C6	C7	0.00054375042844
C1	C8	0.0063169577679
Si2	C8	0.011608482126
C3	C8	0.0074802311857
C4	C8	1.0178031674
C5	C8	0.0053109317391
C6	C8	0.00068700578454
C7	C8	0.00046039514877
C1	C9	0.0073377956702
Si2	C9	0.01125609213

C3	C9	0.002553348233
C4	C9	0.0070817421079
C5	C9	1.0178628477
C6	C9	0.0010365769608
C7	C9	0.0025233286999
C8	C9	0.0011016064723
C1	C1	0.9924790422
Si2	C1	0.012337244174
C3	C1	0.0075665093398
C4	C1	0.0028951566312
C5	C1	0.0061795848986
C6	C1	0.043873267623
C7	C1	0.0010340336748
C8	C1	0.0043641819134
C9	C1	0.00043820901074
C1	H11	0.99575105673
Si2	H11	0.012650268464
C3	H11	0.0047667683792
C4	H11	0.0074808174812
C5	H11	0.0058528087742
C6	H11	0.044252033784
C7	H11	0.00037235480801
C8	H11	0.00052142166544
C9	H11	0.00060003758257
C1	H11	0.046037943661
C1	H12	0.0060911712824
Si2	H12	0.012731092234
C3	H12	0.99584902802
C4	H12	0.0076397501169
C5	H12	0.0041224757035
C6	H12	0.00056731590711
C7	H12	0.04414459532
C8	H12	0.0010071280334
C9	H12	0.00021068025054
C1	H12	0.00049179784849
H11	H12	0.0027200793501
C1	H13	0.0037871544311
Si2	H13	0.012764504608
C3	H13	0.99186662726
C4	H13	0.0048740899874
C5	H13	0.0074711195636
C6	H13	0.0057305301769
C7	H13	0.043937501716
C8	H13	0.00037577183981
C9	H13	0.00019106968266
C1	H13	0.0002044380331
H11	H13	0.000235147379
H12	H13	0.046171315056

C1	H14	0.0074606576668
Si2	H14	0.012482216661
C3	H14	0.0031867106137
C4	H14	0.99134133683
C5	H14	0.0031560353003
C6	H14	0.00044155814743
C7	H14	0.0040249138138
C8	H14	0.043539697664
C9	H14	0.0047392762114
C1	H14	0.00022415617234
H11	H14	0.00098123797405
H12	H14	0.00017884569349
H13	H14	0.00022974760504
C1	H15	0.0028006699333
Si2	H15	0.012610762902
C3	H15	0.0058183173875
C4	H15	0.99367429364
C5	H15	0.0075207852388
C6	H15	0.0035133580972
C7	H15	0.00048828803693
C8	H15	0.043898922587
C9	H15	0.00057985742267
C1	H15	0.00013995307332
H11	H15	0.00021972687404
H12	H15	0.00047761720287
H13	H15	0.002664675676
H14	H15	0.045542224849
C1	H16	0.0088108788612
Si2	H16	0.012556152547
C3	H16	0.0073430498671
C4	H16	0.0024322352252
C5	H16	0.99315659719
C6	H16	0.00087480668085
C7	H16	0.00021896069152
C8	H16	0.0022741512896
C9	H16	0.044001452074
C1	H16	0.0048423900141
H11	H16	0.00068353349017
H12	H16	0.00028758223409
H13	H16	0.0010095771463
H14	H16	0.00014005923962
H15	H16	0.00023795834983
C1	H17	0.0043112542434
Si2	H17	0.012825705213
C3	H17	0.0058122461865
C4	H17	0.007256271353
C5	H17	0.9965304411
C6	H17	0.00033138190096

C7	H17	0.00047610305066
C8	H17	0.00041268613603
C9	H17	0.0440716205
C1	H17	0.00038810413924
H11	H17	0.0023167683287
H12	H17	0.0021450591184
H13	H17	0.00047066178358
H14	H17	0.00021146413052
H15	H17	0.00094516056713
H16	H17	0.046271293817
C1	H18	0.045108212842
Si2	H18	0.0010710790129
C3	H18	0.0071169098962
C4	H18	0.00037730322878
C5	H18	0.0003217898849
C6	H18	0.96081826161
C7	H18	0.00099534609592
C8	H18	7.3996179176e-05
C9	H18	3.0447721333e-05
C1	H18	0.011538728485
H11	H18	0.0035232801744
H12	H18	0.00084849669774
H13	H18	0.0096735010215
H14	H18	2.7364906898e-05
H15	H18	0.00024418501189
H16	H18	0.00016979099882
H17	H18	1.8477832598e-05
C1	H19	0.045373666329
Si2	H19	0.00117741439
C3	H19	0.00043863783469
C4	H19	0.005850457044
C5	H19	0.00034748236825
C6	H19	0.96096843862
C7	H19	3.4301448417e-05
C8	H19	0.0020408983405
C9	H19	3.4578600113e-05
C1	H19	0.0031547998518
H11	H19	0.011702355294
H12	H19	8.3864065381e-05
H13	H19	0.00041341020364
H14	H19	0.00074886172121
H15	H19	0.0060559854688
H16	H19	3.7811176329e-05
H17	H19	9.6402949031e-05
H18	H19	0.045091460312
C1	Si2	0.051095705835
Si2	Si2	0.0043535239966
C3	Si2	0.00091074699978

C4	Si2	0.00083179758123
C5	Si2	0.0018195592673
C6	Si2	0.96363448628
C7	Si2	7.2772963189e-05
C8	Si2	5.5620968387e-05
C9	Si2	0.00027419122578
C1	Si2	0.0044211088545
H11	Si2	0.0041494342636
H12	Si2	5.5458646147e-05
H13	Si2	0.00081572131441
H14	Si2	6.9297889077e-05
H15	Si2	0.0005504495151
H16	Si2	5.7087511715e-05
H17	Si2	3.6263537819e-05
H18	Si2	0.044404846187
H19	Si2	0.044611453292
C1	H21	0.0018277877891
Si2	H21	0.0043436089446
C3	H21	0.051223907217
C4	H21	0.00078439511185
C5	H21	0.00061032237484
C6	H21	4.7397629002e-05
C7	H21	0.96345415406
C8	H21	6.6833358531e-05
C9	H21	0.00033872941063
C1	H21	0.00031363444583
H11	H21	4.2370758905e-05
H12	H21	0.0038934900766
H13	H21	0.0049015713831
H14	H21	0.00053648033878
H15	H21	4.6229810539e-05
H16	H21	7.4289849142e-05
H17	H21	5.2250385089e-05
H18	H21	3.6363472224e-05
H19	H21	5.6922222275e-06
Si2	H21	2.245127215e-05
C1	H22	0.0002812130866
Si2	H22	0.0009235506743
C3	H22	0.045353389986
C4	H22	0.0003409458101
C5	H22	0.0023090865025
C6	H22	0.00010285558236
C7	H22	0.95865244663
C8	H22	2.7721730896e-05
C9	H22	0.0068670376555
C1	H22	2.8236766777e-05
H11	H22	1.6420966294e-05
H12	H22	0.0038640673533

H13	H22	0.01128397252
H14	H22	0.000217988444
H15	H22	6.9046517016e-05
H16	H22	0.00028603596406
H17	H22	0.00060958847545
H18	H22	0.00024469042311
H19	H22	6.7926341206e-06
Si2	H22	2.3006333462e-05
H21	H22	0.044041897042
C1	H23	0.00033978147786
Si2	H23	0.001207298442
C3	H23	0.045668609521
C4	H23	0.0063073905546
C5	H23	0.00032980365245
C6	H23	2.227784479e-05
C7	H23	0.96120655873
C8	H23	0.00093311670135
C9	H23	0.0004175493794
C1	H23	3.0310015245e-05
H11	H23	0.00010399833502
H12	H23	0.011703726734
H13	H23	0.0030234659134
H14	H23	0.0074533687845
H15	H23	0.00073331367534
H16	H23	3.5382742489e-05
H17	H23	6.5395010533e-05
H18	H23	5.2659187158e-05
H19	H23	4.5636356773e-06
Si2	H23	3.4386724735e-06
H21	H23	0.044519701604
H22	H23	0.044893079408
C1	H24	0.00089610690183
Si2	H24	0.0043653197418
C3	H24	0.0019194512211
C4	H24	0.051056261261
C5	H24	0.00083465801685
C6	H24	5.5254302481e-05
C7	H24	4.9779366361e-05
C8	H24	0.96355589649
C9	H24	7.7044979582e-05
C1	H24	0.00069398757713
H11	H24	6.8797998532e-05
H12	H24	0.00032891243263
H13	H24	4.345660028e-05
H14	H24	0.0044049182682
H15	H24	0.004073369396
H16	H24	0.00038155820378
H17	H24	6.9494815963e-05

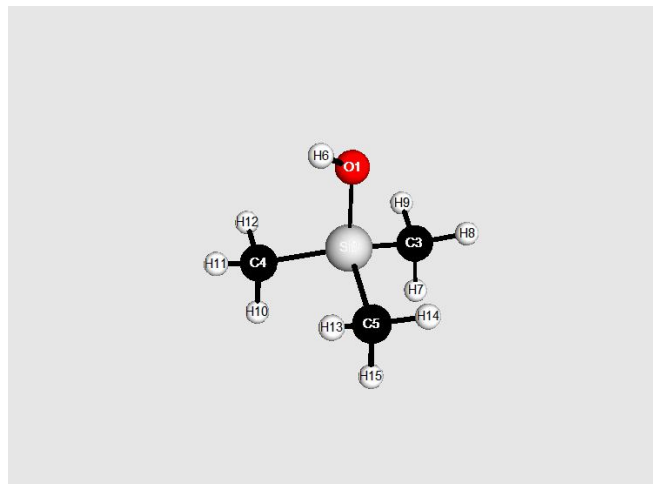
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H19	H24	0.00013649580299
Si2	H24	2.8466270397e-06
H21	H24	2.1834392305e-05
H22	H24	5.0653672199e-06
H23	H24	3.7053934749e-05
C1	H25	0.00050169498039
Si2	H25	0.0012129322195
C3	H25	0.00033992971806
C4	H25	0.045262690071
C5	H25	0.0053787682627
C6	H25	7.392139865e-05
C7	H25	1.9680091415e-05
C8	H25	0.96015189812
C9	H25	0.0034477267711
C1	H25	0.00042696081731
H11	H25	3.8968342883e-05
H12	H25	3.2754847234e-05
H13	H25	0.00010075838152
H14	H25	0.0030387527886
H15	H25	0.011612894077
H16	H25	0.0040143447535
H17	H25	0.0007057313975
H18	H25	2.1783303438e-05
H19	H25	0.00024746163991
Si2	H25	5.6170807999e-06
H21	H25	3.5288189432e-06
H22	H25	6.2163730623e-06
H23	H25	4.7078616895e-05
H24	H25	0.044539618002
C1	H26	0.006497248578
Si2	H26	0.0011054212993
C3	H26	0.00029271216924
C4	H26	0.044997423363
C5	H26	0.00036298884493
C6	H26	0.0021131206791
C7	H26	7.603954531e-05
C8	H26	0.960123079
C9	H26	0.00011470960434
C1	H26	0.0069779479429
H11	H26	0.00083027041486
H12	H26	3.3281518285e-05
H13	H26	1.7766328727e-05
H14	H26	0.011369841098
H15	H26	0.0034180292864
H16	H26	0.00015060137522
H17	H26	2.4502644942e-05
H18	H26	0.00027193043135

H19	H26	0.0033780428633
Si2	H26	0.00013335480153
H21	H26	1.8353086413e-05
H22	H26	2.9212994083e-06
H23	H26	0.00020624052547
H24	H26	0.044320712798
H25	H26	0.044882805807
C1	H27	0.0017552722443
Si2	H27	0.0043593732675
C3	H27	0.00065440463109
C4	H27	0.00093340208629
C5	H27	0.05119370378
C6	H27	0.00027031602909
C7	H27	0.00029052979335
C8	H27	8.2046911128e-05
C9	H27	0.96376116697
C1	H27	3.3734095929e-05
H11	H27	3.8319592654e-05
H12	H27	2.4137237545e-05
H13	H27	0.00011957446473
H14	H27	0.00078548642218
H15	H27	6.5841713098e-05
H16	H27	0.0044111991249
H17	H27	0.0042890570341
H18	H27	9.1928612186e-06
H19	H27	1.0751395817e-05
Si2	H27	9.6304612074e-05
H21	H27	5.6673253842e-05
H22	H27	0.00059967435022
H23	H27	7.4818386202e-05
H24	H27	3.7717010494e-06
H25	H27	0.00024239526859
H26	H27	7.7811732631e-06
C1	H28	0.00031900490016
Si2	H28	0.0010970439378
C3	H28	0.00024870298849
C4	H28	0.0063628218109
C5	H28	0.044981866071
C6	H28	3.26573069e-05
C7	H28	0.00014055400529
C8	H28	0.0036621014058
C9	H28	0.95871920793
C1	H28	2.5465343653e-05
H11	H28	0.00010629733004
H12	H28	6.3019949578e-05
H13	H28	1.7311686435e-05
H14	H28	0.0063346517008
H15	H28	0.00080680241014



H16	H28	0.0033458966186
H17	H28	0.011577120794
H18	H28	1.755419141e-06
H19	H28	1.2412058396e-05
Si2	H28	1.0448888117e-05
H21	H28	1.5556014095e-05
H22	H28	0.00048044830957
H23	H28	5.2751596513e-05
H24	H28	0.0002270374315
H25	H28	0.0063520136816
H26	H28	0.00041179798205
H27	H28	0.044297743374
C1	H29	0.0003388770735
Si2	H29	0.00098542620601
C3	H29	0.0011186970072
C4	H29	0.0007060966359
C5	H29	0.045316903255
C6	H29	3.481576936e-05
C7	H29	0.0082929808696
C8	H29	0.00012470923068
C9	H29	0.95841417558
C1	H29	0.00013978926643
H11	H29	2.7885116646e-05
H12	H29	6.4613845434e-05
H13	H29	0.00016035901235
H14	H29	0.00076769637771
H15	H29	5.6758305708e-05
H16	H29	0.011574825629
H17	H29	0.0033041740926
H18	H29	7.0099437095e-06
H19	H29	1.9455485322e-06
Si2	H29	9.5306206671e-06
H21	H29	0.0011452573194
H22	H29	0.014526995847
H23	H29	0.0011281780435
H24	H29	7.6852622245e-06
H25	H29	0.00035184317753
H26	H29	3.4019400695e-05
H27	H29	0.044254692169
H28	H29	0.044662488728

## TRIMETHYLSILANOL



## HARTREE-FOCK

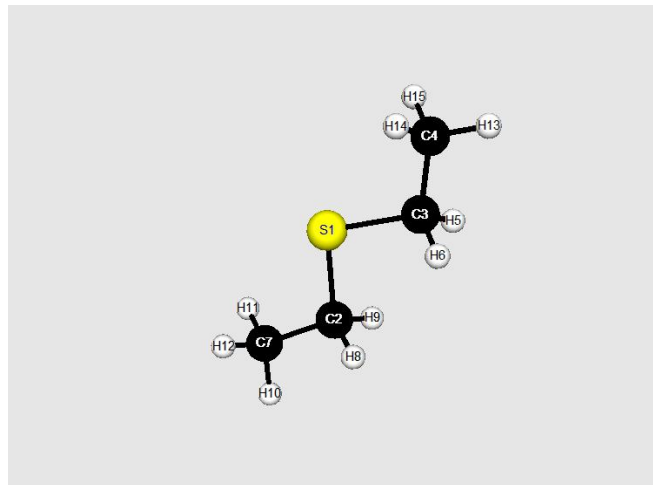
Atom A	Atom B	Delocalization index
O1	Si2	0.34361318253
O1	C3	0.1017405242
Si2	C3	0.40060665872
O1	C4	0.1088321574
Si2	C4	0.39494604619
C3	C4	0.09462375403
O1	C5	0.10903853967
Si2	C5	0.39482842773
C3	C5	0.094539587188
C4	C5	0.099193623571
O1	H6	0.59552441591
Si2	H6	0.0052115484594
C3	H6	0.0054669189432
C4	H6	0.00093462724445
C5	H6	0.00095504539785
O1	H7	0.0078758648703
Si2	H7	0.012657400993
C3	H7	1.0146069408
C4	H7	0.0042854431485
C5	H7	0.0042648031715
H6	H7	0.00078534236717
O1	H8	0.0057935626655
Si2	H8	0.011999641558
C3	H8	1.0096738652
C4	H8	0.0082730189889
C5	H8	0.0044815323758
H6	H8	0.00012984124178
H7	H8	0.044288629728
O1	H9	0.005783623687
Si2	H9	0.012045800869

C3	H9	1.0095791491
C4	H9	0.0044780605148
C5	H9	0.0082667522071
H6	H9	0.00013141013641
H7	H9	0.044293895727
H8	H9	0.04348231095
O1	O1	0.0095489933079
Si2	O1	0.012165658784
C3	O1	0.0041021714186
C4	O1	1.0123858129
C5	O1	0.0046470419946
H6	O1	7.2384637517e-05
H7	O1	0.0014115594639
H8	O1	0.00034804771231
H9	O1	0.00021115553391
O1	H11	0.0054356487345
Si2	H11	0.012236958
C3	H11	0.0084832870798
C4	H11	1.0128076598
C5	H11	0.0049063203632
H6	H11	0.00023716916759
H7	H11	0.00037334197512
H8	H11	0.0013337232457
H9	H11	0.00035761757687
O1	H11	0.045401470771
O1	H12	0.005706092969
Si2	H12	0.011761782167
C3	H12	0.0046104358001
C4	H12	1.0097399298
C5	H12	0.008621084036
H6	H12	3.5431242137e-05
H7	H12	0.00021586657635
H8	H12	0.00037599954621
H9	H12	0.0016142305815
O1	H12	0.044340161689
H11	H12	0.044700628595
O1	H13	0.0054513868636
Si2	H13	0.012243994372
C3	H13	0.0084768200517
C4	H13	0.0049032434933
C5	H13	1.0127911288
H6	H13	0.00025042095504
H7	H13	0.00037098777169
H8	H13	0.00035836608511
H9	H13	0.0013326335859
O1	H13	0.00024255672176
H11	H13	0.0018149776138
H12	H13	0.00039872089412

O1	H14	0.0057137812469
Si2	H14	0.011704453122
C3	H14	0.0046061071205
C4	H14	0.0086244625519
C5	H14	1.0097727164
H6	H14	3.5698395489e-05
H7	H14	0.00021491124071
H8	H14	0.0016173887598
H9	H14	0.00037557807418
O1	H14	0.00039507833836
H11	H14	0.0003994824302
H12	H14	0.0013747037874
H13	H14	0.044709224656
O1	H15	0.0095641258292
Si2	H15	0.012183823555
C3	H15	0.0040914212497
C4	H15	0.0046610328776
C5	H15	1.0123237627
H6	H15	7.4410587602e-05
H7	H15	0.0013999160288
H8	H15	0.00021062657028
H9	H15	0.00034751393898
O1	H15	0.0017243646423
H11	H15	0.0002427942092
H12	H15	0.00039645704802
H13	H15	0.045406080089
H14	H15	0.044337471247

# SULFIDES AND THIOLS

## DIETHYL SULFIDE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
S1	C2	1.0691261898
S1	C3	1.0691697384
C2	C3	0.039822776304
S1	C4	0.062792501631
C2	C4	0.0092623503814
C3	C4	0.98882494835
S1	H5	0.062739739735
C2	H5	0.0059426037674
C3	H5	0.95110674608
C4	H5	0.038889273136
S1	H6	0.062669797676
C2	H6	0.0059471891864
C3	H6	0.95105900351
C4	H6	0.038855792705
H5	H6	0.038407520921
S1	C7	0.062913971416
C2	C7	0.98883631751
C3	C7	0.0092763254654
C4	C7	0.0016078543179
H5	C7	0.00075323978102
H6	C7	0.00075354525808
S1	H8	0.062682745163
C2	H8	0.95090437815
C3	H8	0.0059550549198
C4	H8	0.00075294188417
H5	H8	0.00041134533349
H6	H8	0.0053264602367
C7	H8	0.038891707126

S1	H9	0.062748386703
C2	H9	0.9508612708
C3	H9	0.0059556766728
C4	H9	0.00075264656297
H5	H9	0.0053262864599
H6	H9	0.00041139132091
C7	H9	0.038887079298
H8	H9	0.038437164598
S1	S1	0.014856246685
C2	S1	0.04490072306
C3	S1	0.0022995645525
C4	S1	0.00049841301806
H5	S1	5.9983078731e-05
H6	S1	5.9984865146e-05
C7	S1	0.9633810897
H8	S1	0.003575548747
H9	S1	0.0035754744166
S1	H11	0.015818459769
C2	H11	0.043144028923
C3	H11	0.00095474079343
C4	H11	6.8933325253e-05
H5	H11	5.2260465828e-05
H6	H11	0.00037058459223
C7	H11	0.96064976131
H8	H11	0.01093694603
H9	H11	0.0033960174047
S1	H11	0.041695085595
S1	H12	0.015821173399
C2	H12	0.043190511962
C3	H12	0.00095473230624
C4	H12	6.8945476463e-05
H5	H12	0.00037058490184
H6	H12	5.2266917196e-05
C7	H12	0.96063957889
H8	H12	0.0033960890562
H9	H12	0.010936924866
S1	H12	0.041694664442
H11	H12	0.041669852505
S1	H13	0.014857266393
C2	H13	0.0022987607863
C3	H13	0.044938624096
C4	H13	0.96327878172
H5	H13	0.0035714958661
H6	H13	0.0035715966991
C7	H13	0.0004989427414
H8	H13	5.9953306423e-05
H9	H13	5.9952949688e-05
S1	H13	0.00021909692718

H11	H13	2.9765967641e-05
H12	H13	2.9766406231e-05
S1	H14	0.015829480264
C2	H14	0.00095465930229
C3	H14	0.043155322866
C4	H14	0.9605420442
H5	H14	0.010930890725
H6	H14	0.0033953868014
C7	H14	6.9101162569e-05
H8	H14	5.2343496126e-05
H9	H14	0.00037082234456
S1	H14	2.9784292206e-05
H11	H14	8.03620828e-06
H12	H14	2.5372810493e-05
H13	H14	0.041692879885
S1	H15	0.015826698453
C2	H15	0.00095479425998
C3	H15	0.043239005098
C4	H15	0.96053225561
H5	H15	0.0033953455721
H6	H15	0.010930900884
C7	H15	6.9107911479e-05
H8	H15	0.00037082058911
H9	H15	5.2340737451e-05
S1	H15	2.9783566597e-05
H11	H15	2.5371927163e-05
H12	H15	8.0363087517e-06
H13	H15	0.041692670726
H14	H15	0.041665189084

#### CCSD

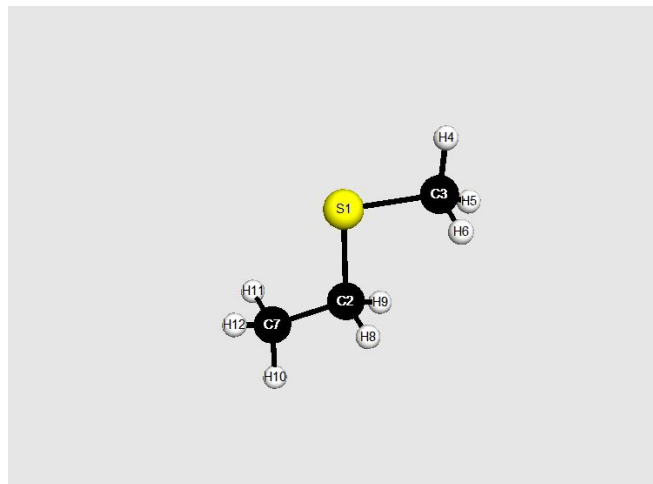
Atom A	Atom B	Delocalization index
C1	S2	0.8835902305
C1	C3	0.84813505651
S2	C3	0.055073181017
C1	C4	0.034861118441
S2	C4	0.88360943792
C3	C4	0.0071277021192
C1	C5	0.0071310542925
S2	C5	0.055097849319
C3	C5	0.0013735250946
C4	C5	0.84815667508
C1	H6	0.81371004461
S2	H6	0.049631204927
C3	H6	0.031949431365
C4	H6	0.0061120093334
C5	H6	0.00069671567409
C1	H7	0.81352912399

S2	H7	0.049660062367
C3	H7	0.031953625352
C4	H7	0.0061092313506
C5	H7	0.00069600641902
H6	H7	0.030516654777
C1	H8	0.035339497874
S2	H8	0.011554103418
C3	H8	0.82878297942
C4	H8	0.0018881610874
C5	H8	0.00045074633737
H6	H8	0.0031532635124
H7	H8	0.0031535566427
C1	H9	0.03422736866
S2	H9	0.016056989076
C3	H9	0.8255043696
C4	H9	0.00083195985999
C5	H9	7.611972875e-05
H6	H9	0.0088218670501
H7	H9	0.0030049610763
H8	H9	0.032699195078
C1	C1	0.034247052755
S2	C1	0.016059114623
C3	C1	0.82552971989
C4	C1	0.00083191380744
C5	C1	7.6057427823e-05
H6	C1	0.0030047597642
H7	C1	0.0088219302013
H8	C1	0.032698808319
H9	C1	0.032851335491
C1	H11	0.0060995608477
S2	H11	0.049662514341
C3	H11	0.00069582937012
C4	H11	0.81369745504
C5	H11	0.031956206341
H6	H11	0.00050377565587
H7	H11	0.0068279686481
H8	H11	6.9808213526e-05
H9	H11	6.489014309e-05
C1	H11	0.00039635643308
C1	H12	0.0061156130366
S2	H12	0.049620238546
C3	H12	0.00069585280902
C4	H12	0.81339797528
C5	H12	0.031953312895
H6	H12	0.0068369585005
H7	H12	0.00050375882591
H8	H12	6.9786194295e-05
H9	H12	0.00039645931499



C1	H12	6.4899502631e-05
H11	H12	0.030516580156
C1	H13	0.0018882781715
S2	H13	0.011554107103
C3	H13	0.00045063555433
C4	H13	0.035339131726
C5	H13	0.82882117283
H6	H13	6.9789883347e-05
H7	H13	6.9810149338e-05
H8	H13	0.00022753757474
H9	H13	3.3763175979e-05
C1	H13	3.3737891925e-05
H11	H13	0.0031536248956
H12	H13	0.0031534571484
C1	H14	0.00083129082667
S2	H14	0.016059433775
C3	H14	7.6030738781e-05
C4	H14	0.034264282756
C5	H14	0.82549363341
H6	H14	6.4909978701e-05
H7	H14	0.00039638723681
H8	H14	3.373879275e-05
H9	H14	1.3757287131e-05
C1	H14	3.651331149e-05
H11	H14	0.0088218551957
H12	H14	0.0030047602169
H13	H14	0.032698850449
C1	H15	0.00083204635837
S2	H15	0.016055964515
C3	H15	7.6035791726e-05
C4	H15	0.034269808445
C5	H15	0.82553785531
H6	H15	0.00039648143152
H7	H15	6.4888230218e-05
H8	H15	3.3760714086e-05
H9	H15	3.6503673251e-05
C1	H15	1.3754466764e-05
H11	H15	0.0030044269877
H12	H15	0.0088216750453
H13	H15	0.032699031092
H14	H15	0.032850831504

## ETHYL METHYL SULFIDE

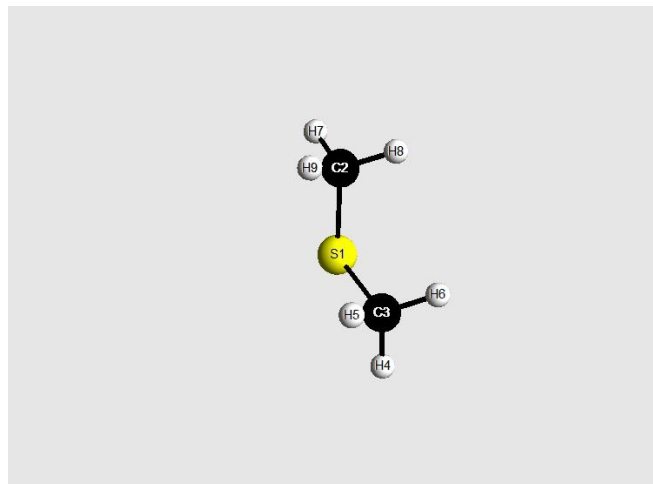


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
S1	C2	1.0695989597
S1	C3	1.0977927429
C2	C3	0.042544034274
S1	H4	0.051893601404
C2	H4	0.0099870965722
C3	H4	0.96640432894
S1	H5	0.063335092404
C2	H5	0.0055302664603
C3	H5	0.96366314781
H4	H5	0.037806449575
S1	H6	0.06318792288
C2	H6	0.0055261470552
C3	H6	0.96361087973
H4	H6	0.03780707591
H5	H6	0.038622422167
S1	C7	0.062567027639
C2	C7	0.98903760995
C3	C7	0.0096308870552
H4	C7	0.0018667183049
H5	C7	0.0007069920768
H6	C7	0.00070696511519
S1	H8	0.0629732603
C2	H8	0.9508972735
C3	H8	0.0062353761657
H4	H8	0.00070258415609
H5	H8	0.00038971685393
H6	H8	0.0047196919004
C7	H8	0.038812151555
S1	H9	0.063131265625
C2	H9	0.9509105002

C3	H9	0.0062380895316
H4	H9	0.00070259975709
H5	H9	0.0047199190065
H6	H9	0.00038970883276
C7	H9	0.038820943231
H8	H9	0.038406503696
S1	S1	0.014877463861
C2	S1	0.044899616741
C3	S1	0.0024012106414
H4	S1	0.0005871873098
H5	S1	7.8529279355e-05
H6	S1	7.8528289384e-05
C7	S1	0.96331479415
H8	S1	0.00356260621
H9	S1	0.003562503369
S1	H11	0.015771864144
C2	H11	0.043200519314
C3	H11	0.00097688914532
H4	H11	6.310888637e-05
H5	H11	5.3338247681e-05
H6	H11	0.00036340700666
C7	H11	0.96045667808
H8	H11	0.010948247772
H9	H11	0.0033931158744
S1	H11	0.041657113836
S1	H12	0.015778112797
C2	H12	0.043186274529
C3	H12	0.00097705687858
H4	H12	6.3108561762e-05
H5	H12	0.00036341874703
H6	H12	5.3336089805e-05
C7	H12	0.96045326943
H8	H12	0.0033930623049
H9	H12	0.010948274962
S1	H12	0.041657379452
H11	H12	0.041637293722

## DIMETHYL SULFIDE



### HARTREE-FOCK

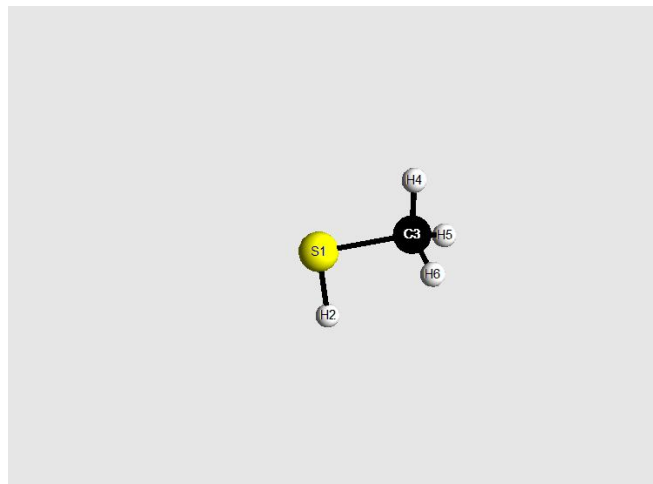
Atom A	Atom B	Delocalization index
S1	C2	1.0987956412
S1	C3	1.0984255384
C2	C3	0.045455094233
S1	H4	0.051705732941
C2	H4	0.010399564633
C3	H4	0.96653848021
S1	H5	0.063612192557
C2	H5	0.0057802482377
C3	H5	0.96373542001
H4	H5	0.037734715992
S1	H6	0.063545670739
C2	H6	0.0057866591541
C3	H6	0.96378072493
H4	H6	0.037734428929
H5	H6	0.038581220969
S1	H7	0.051692073491
C2	H7	0.96658256308
C3	H7	0.010414574929
H4	H7	0.0021727519225
H5	H7	0.0006453398871
H6	H7	0.00064536902029
S1	H8	0.063555922206
C2	H8	0.96367641272
C3	H8	0.0057878390665
H4	H8	0.00064493586674
H5	H8	0.00037230926374
H6	H8	0.0041798893838
H7	H8	0.037731978809
S1	H9	0.063618218697
C2	H9	0.96364387301

C3	H9	0.0057820507751
H4	H9	0.00064489369923
H5	H9	0.0041797712124
H6	H9	0.00037230309012
H7	H9	0.037731649092
H8	H9	0.038591143314

#### CCSD

Atom A	Atom B	Delocalization index
C1	S2	0.9102284214
C1	C3	0.0399747137
S2	C3	0.91010391568
C1	H4	0.8263115476
S2	H4	0.05018986887
C3	H4	0.0060063480162
C1	H5	0.82621881053
S2	H5	0.050163269929
C3	H5	0.0060160695706
H4	H5	0.030787550385
C1	H6	0.83076167475
S2	H6	0.04153807182
C3	H6	0.0080104528242
H4	H6	0.030187984956
H5	H6	0.030186909738
C1	H7	0.0080130553034
S2	H7	0.041537385742
C3	H7	0.83073870626
H4	H7	0.00063349605688
H5	H7	0.00063380843999
H6	H7	0.00201420665
C1	H8	0.0060233875948
S2	H8	0.050153960035
C3	H8	0.82617996388
H4	H8	0.00046299233102
H5	H8	0.0054520974081
H6	H8	0.0006337800256
H7	H8	0.030187378011
C1	H9	0.0060111660928
S2	H9	0.050192625957
C3	H9	0.82624249774
H4	H9	0.0054430199711
H5	H9	0.00046297357789
H6	H9	0.00063343790912
H7	H9	0.030188237752
H8	H9	0.030787419234

## METHANETHIOL



### HARTREE-FOCK

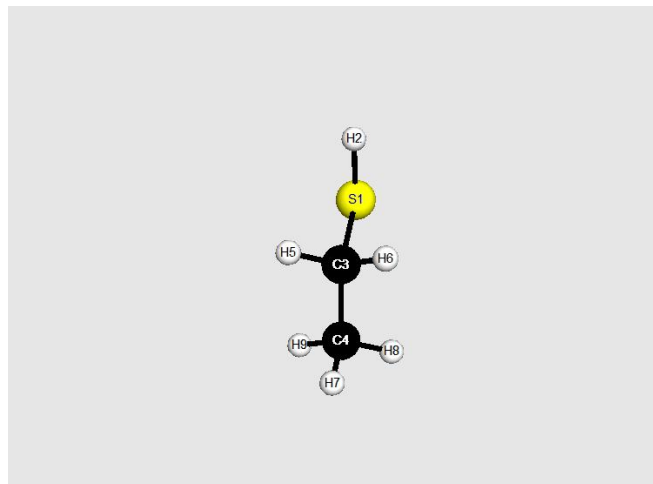
Atom A	Atom B	Delocalization index
S1	H2	1.1390621143
S1	C3	1.0958467432
H2	C3	0.047721891778
S1	H4	0.053365422588
H2	H4	0.010934869712
C3	H4	0.96647380836
S1	H5	0.063847099967
H2	H5	0.0033624209674
C3	H5	0.96671608386
H4	H5	0.037543887438
S1	H6	0.06384726592
H2	H6	0.0033624643334
C3	H6	0.96675343062
H4	H6	0.037543541537
H5	H6	0.037409395135

### CCSD

Atom A	Atom B	Delocalization index
S1	H2	0.9499299577
S1	C3	0.91058130129
H2	C3	0.038202230941
S1	H4	0.043036501623
H2	H4	0.0084575479802
C3	H4	0.83048067012
S1	H5	0.050369040122
H2	H5	0.0030980847059
C3	H5	0.83057319103
H4	H5	0.030155636269
S1	H6	0.050367977612
H2	H6	0.0030981895208

C3	H6	0.83055218267
H4	H6	0.030155771211
H5	H6	0.0299360601

## ETHANETHIOL



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
S1	H2	1.1389041101
S1	C3	1.0646112432
H2	C3	0.045003921391
S1	C4	0.064801573625
H2	C4	0.010379294479
C3	C4	0.98993091974
S1	H5	0.063762029496
H2	H5	0.0034074271371
C3	H5	0.9547741766
C4	H5	0.038632103089
S1	H6	0.063748475728
H2	H6	0.0034074631029
C3	H6	0.95484836402
C4	H6	0.038669110497
H5	H6	0.037253230326
S1	H7	0.015511247943
H2	H7	0.0027107160159
C3	H7	0.044953613151
C4	H7	0.96256383851
H5	H7	0.0034711944074
H6	H7	0.0034712289825
S1	H8	0.015755793312
H2	H8	0.0010255361294
C3	H8	0.04356644777
C4	H8	0.96018242076
H5	H8	0.010968579917
H6	H8	0.0033954034339
H7	H8	0.04133318092
S1	H9	0.01575460639
H2	H9	0.0010255002993



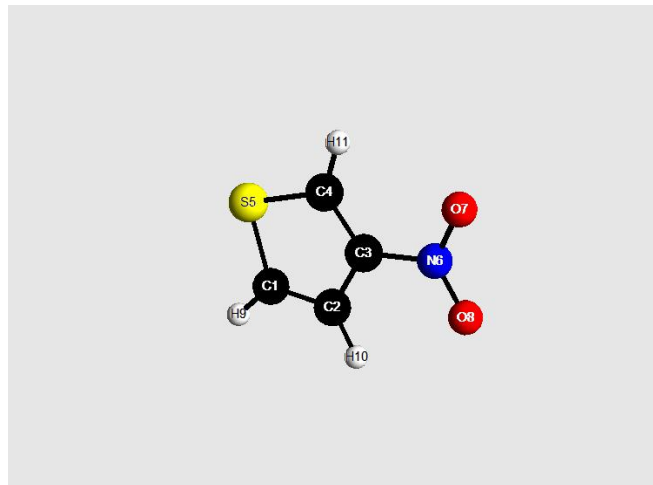
C3	H9	0.043339754134
C4	H9	0.96032804439
H5	H9	0.0033953793643
H6	H9	0.010968578616
H7	H9	0.041333122536
H8	H9	0.041494749528

### CCSD

Atom A	Atom B	Delocalization index
S1	H2	0.94888342579
S1	C3	0.8827733683
H2	C3	0.035851736767
S1	C4	0.057466691678
H2	C4	0.0080144668538
C3	C4	0.85056377411
S1	H5	0.050584329123
H2	H5	0.0032124975181
C3	H5	0.81822725447
C4	H5	0.032075814153
S1	H6	0.050584910076
H2	H6	0.0032125671547
C3	H6	0.81819569126
C4	H6	0.032003942487
H5	H6	0.029685702453
S1	H7	0.012161371756
H2	H7	0.0023489688878
C3	H7	0.035162567756
C4	H7	0.8279677631
H5	H7	0.0030875744225
H6	H7	0.0030876584437
S1	H8	0.016172825173
H2	H8	0.00093964533534
C3	H8	0.034072297868
C4	H8	0.82471694637
H5	H8	0.0089187606432
H6	H8	0.0030134044448
H7	H8	0.032199293637
S1	H9	0.016173094731
H2	H9	0.00093964469399
C3	H9	0.034060731437
C4	H9	0.82469263417
H5	H9	0.0030133869634
H6	H9	0.0089187698381
H7	H9	0.032199282309
H8	H9	0.032524370983

# THIOPHENES

## 3-NITROTHIOPHENE

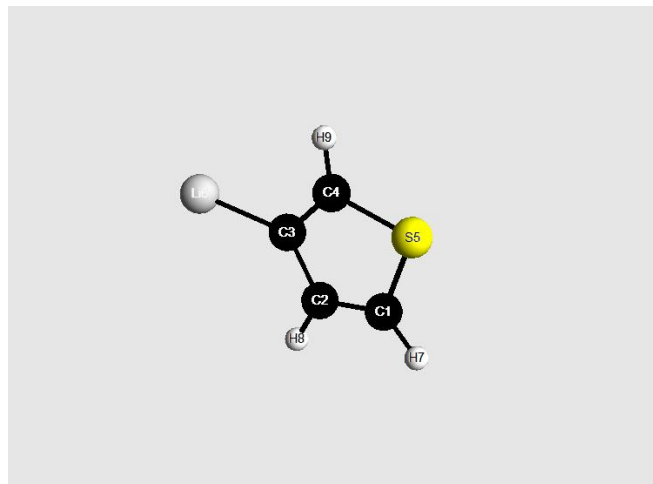


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6148547204
C1	C3	0.095862234732
C2	C3	1.1460315131
C1	C4	0.13593378751
C2	C4	0.078119036608
C3	C4	1.5097144288
C1	S5	1.2395500208
C2	S5	0.13869751598
C3	S5	0.14600493022
C4	S5	1.2942434806
C1	N6	0.010580066457
C2	N6	0.051651219856
C3	N6	0.81309352327
C4	N6	0.086460813667
S5	N6	0.023410130496
C1	O7	0.0055793308664
C2	O7	0.013322285042
C3	O7	0.076234347086
C4	O7	0.049356762085
S5	O7	0.0082061710229
N6	O7	1.6780782093
C1	O8	0.0036207743738
C2	O8	0.033399374509
C3	O8	0.074957670092
C4	O8	0.027377927708
S5	O8	0.012039667887
N6	O8	1.6844806854
O7	O8	0.32233650428

C1	H9	0.97318219044
C2	H9	0.046601931901
C3	H9	0.0094658107617
C4	H9	0.012858890396
S5	H9	0.042576699756
N6	H9	0.0013728830902
O7	H9	0.00088187207309
O8	H9	0.00014292263233
C1	C1	0.04959582535
C2	C1	0.95094313548
C3	C1	0.034580919371
C4	C1	0.0072623888028
S5	C1	0.017038341311
N6	C1	0.0029358349495
O7	C1	0.0010649994965
O8	C1	0.019833780966
H9	C1	0.0036724017803
C1	H11	0.012207143392
C2	H11	0.0079871214825
C3	H11	0.039609654096
C4	H11	0.94642444401
S5	H11	0.037283902923
N6	H11	0.0043929018824
O7	H11	0.019336068126
O8	H11	0.0017090702392
H9	H11	0.0016388499589
C1	H11	0.0012262301221

### 3-LITHIUMTHIOPHENE

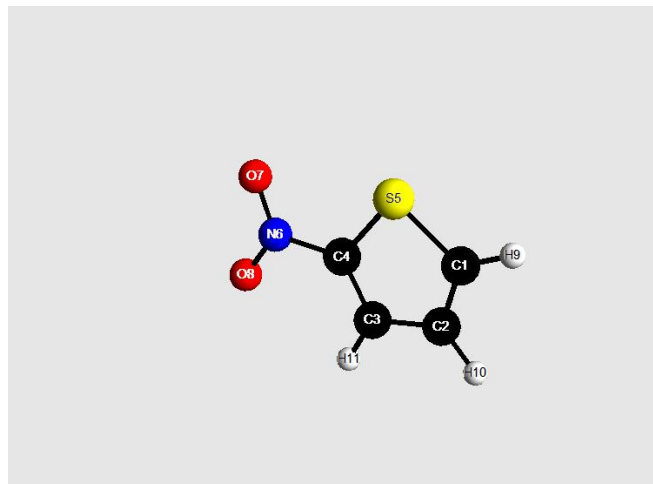


#### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6116376854
C1	C3	0.09100405615
C2	C3	1.1996533384
C1	C4	0.14098311648
C2	C4	0.11334184769
C3	C4	1.6782651095
C1	S5	1.2537309853
C2	S5	0.15916685444
C3	S5	0.1758307694
C4	S5	1.2170191803
C1	Li6	0.0017605583653
C2	Li6	0.0057308581805
C3	Li6	0.15416489738
C4	Li6	0.0096944508078
S5	Li6	0.0043782559857
C1	H7	0.98625237058
C2	H7	0.049798167785
C3	H7	0.012228053627
C4	H7	0.015441304072
S5	H7	0.046240097323
Li6	H7	0.00032639443659
C1	H8	0.066982405377
C2	H8	0.9810243548
C3	H8	0.045935919611
C4	H8	0.010390410538
S5	H8	0.022402430985
Li6	H8	0.00051497287951
H7	H8	0.0043772609423
C1	H9	0.015579949544
C2	H9	0.012535817856

C3	H9	0.060195444731
C4	H9	0.99169990708
S5	H9	0.053518912245
Li6	H9	0.00081627372622
H7	H9	0.0021626317645
H8	H9	0.0016457365092

## 2-NITROTHIOPHENE

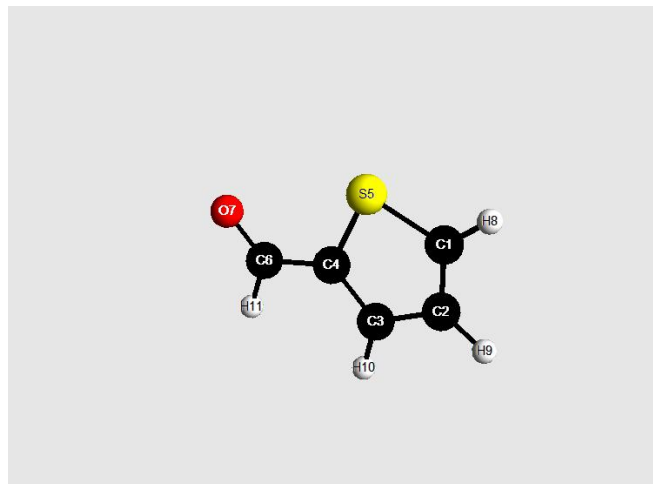


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.5795820332
C1	C3	0.089457462986
C2	C3	1.202086131
C1	C4	0.13719191003
C2	C4	0.089949233758
C3	C4	1.4953831633
C1	S5	1.2734543956
C2	S5	0.14110834724
C3	S5	0.14585301212
C4	S5	1.1956954155
C1	N6	0.020731136099
C2	N6	0.011503873242
C3	N6	0.076475626429
C4	N6	0.85253304407
S5	N6	0.056024109177
C1	O7	0.011643843153
C2	O7	0.0057258172638
C3	O7	0.02634787843
C4	O7	0.084535076446
S5	O7	0.057716925922
N6	O7	1.6753300364
C1	O8	0.011292498537
C2	O8	0.0039030912482
C3	O8	0.04531303461
C4	O8	0.081753634988
S5	O8	0.016965100583
N6	O8	1.6781651642
O7	O8	0.31850869033
C1	H9	0.97106450679
C2	H9	0.044438049387

C3	H9	0.0089328295545
C4	H9	0.012715624366
S5	H9	0.043180349314
N6	H9	0.0019674299294
O7	H9	0.00066167689496
O8	H9	0.0012381291986
C1	C1	0.054670150054
C2	C1	0.97158000125
C3	C1	0.039056712017
C4	C1	0.0082131496059
S5	C1	0.017893189658
N6	C1	0.0013121470565
O7	C1	0.00090364700595
O8	C1	0.00015544891929
H9	C1	0.0038286264808
C1	H11	0.0073717562231
C2	H11	0.032702309339
C3	H11	0.94726380739
C4	H11	0.048124060741
S5	H11	0.016082873928
N6	H11	0.0045811650071
O7	H11	0.0018071859927
O8	H11	0.019698043746
H9	H11	0.0012343231268
C1	H11	0.0026407767617

## 2-THIOPHENECARBALDEHYDE



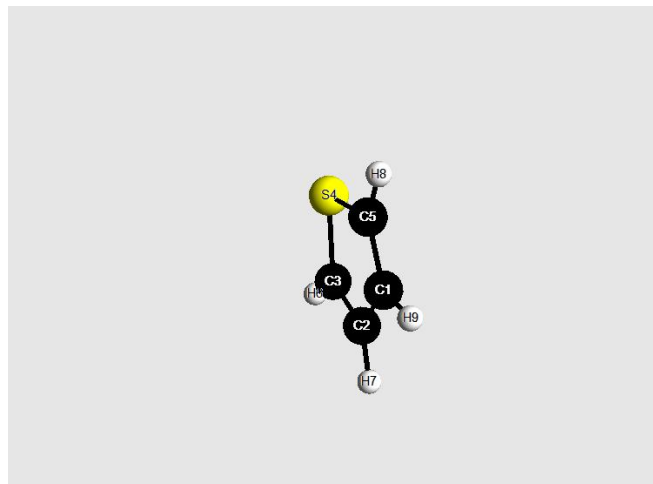
### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.5807766434
C1	C3	0.091490448579
C2	C3	1.2066172983
C1	C4	0.13666412299
C2	C4	0.084930288332
C3	C4	1.5363778708
C1	S5	1.2780061532
C2	S5	0.14404013187
C3	S5	0.1492181984
C4	S5	1.214430649
C1	C6	0.019386300595
C2	C6	0.0097831561358
C3	C6	0.066171299748
C4	C6	1.0064252658
S5	C6	0.040622729916
C1	O7	0.015978948449
C2	O7	0.0063190402167
C3	O7	0.040292047534
C4	O7	0.13680917246
S5	O7	0.041527629874
C6	O7	1.2890327456
C1	H8	0.97418284487
C2	H8	0.045495575389
C3	H8	0.0092328080079
C4	H8	0.013203384869
S5	H8	0.043499140134
C6	H8	0.001904384702
O7	H8	0.0010284197973
C1	H9	0.055775892977
C2	H9	0.97486141898



C3	H9	0.039496102388
C4	H9	0.0084223211697
S5	H9	0.018464651896
C6	H9	0.001077293774
O7	H9	0.00088944023057
H8	H9	0.0038115303867
C1	C1	0.0081897418657
C2	C1	0.037278126716
C3	C1	0.96801466802
C4	C1	0.053052135603
S5	C1	0.019125481043
C6	C1	0.0071253906603
O7	C1	0.0026900863083
H8	C1	0.0013175085757
H9	C1	0.0027235682127
C1	H11	0.0020058978614
C2	H11	0.00090333692628
C3	H11	0.0099797995064
C4	H11	0.052734212743
S5	H11	0.010015409042
C6	H11	0.88479314259
O7	H11	0.11725350249
H8	H11	0.00050713843094
H9	H11	3.702649881e-05
C1	H11	0.0063554889298

# THIOPHENE



## HARTREE-FOCK

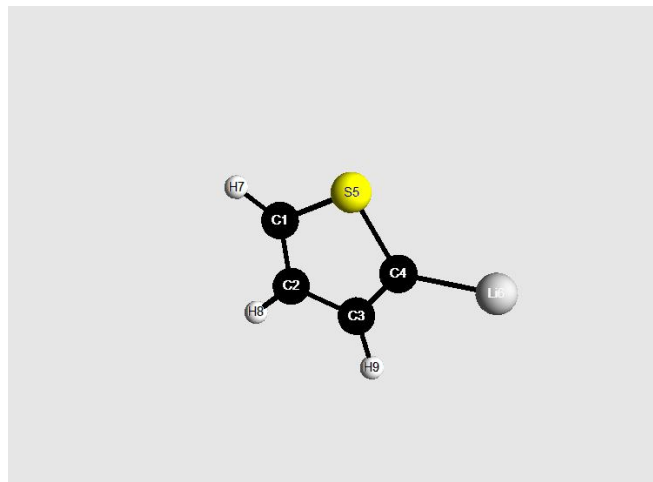
Atom A	Atom B	Delocalization index
C1	C2	1.1834846095
C1	C3	0.090042302305
C2	C3	1.6075381749
C1	S4	0.15113656655
C2	S4	0.15113420937
C3	S4	1.2552166209
C1	C5	1.6075494702
C2	C5	0.090101626163
C3	C5	0.14435257075
S4	C5	1.2554197421
C1	H6	0.0097999577132
C2	H6	0.047388197092
C3	H6	0.97822022632
S4	H6	0.043916322057
C5	H6	0.014219679003
C1	H7	0.038325940184
C2	H7	0.97489657076
C3	H7	0.057577098057
S4	H7	0.019894098146
C5	H7	0.0085462870822
H6	H7	0.0039117258787
C1	H8	0.047393582257
C2	H8	0.0098012598391
C3	H8	0.014220724841
S4	H8	0.043917717843
C5	H8	0.97823497273
H6	H8	0.001903667208
H7	H8	0.0014097690696
C1	H9	0.97492768925
C2	H9	0.038337852308

C3	H9	0.0085455272658
S4	H9	0.019896738855
C5	H9	0.057572911074
H6	H9	0.0014102867798
H7	H9	0.0026990220947
H8	H9	0.0039117862017

### CCSD

Atom A	Atom B	Delocalization index
C1	C2	1.0333815149
C1	C3	0.066460337304
C2	C3	1.2854139052
C1	S4	0.1056815296
C2	S4	0.1056999586
C3	S4	1.0430502007
C1	C5	1.2854125499
C2	C5	0.066492720032
C3	C5	0.099722903066
S4	C5	1.0430441016
C1	H6	0.0076220753053
C2	H6	0.034375876099
C3	H6	0.84502405444
S4	H6	0.034877614579
C5	H6	0.010422683588
C1	H7	0.029962761196
C2	H7	0.84265304443
C3	H7	0.040324623609
S4	H7	0.015334567526
C5	H7	0.0067819649655
H6	H7	0.0029816536941
C1	H8	0.034383410475
C2	H8	0.007622458691
C3	H8	0.010422431243
S4	H8	0.034878394141
C5	H8	0.84496835469
H6	H8	0.0017362286776
H7	H8	0.0013507209476
C1	H9	0.8426489805
C2	H9	0.029968915666
C3	H9	0.0067834453466
S4	H9	0.015335037728
C5	H9	0.040324180806
H6	H9	0.0013507424417
H7	H9	0.0023684977773
H8	H9	0.0029816690532

## 2-LITHIUMTHIOPHENE

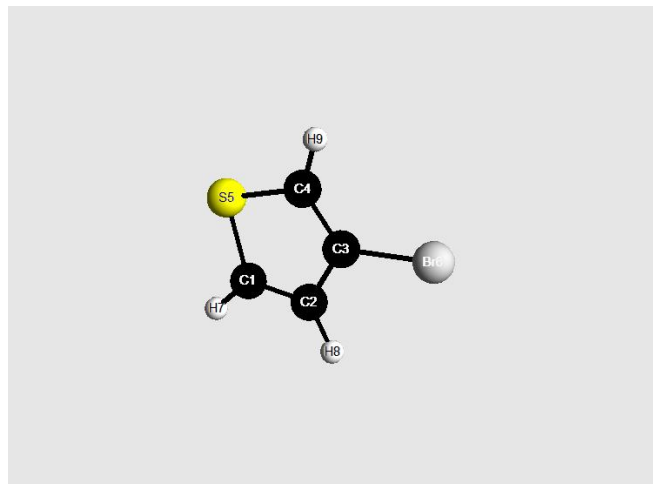


### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6014145428
C1	C3	0.093747795047
C2	C3	1.1911507022
C1	C4	0.15954069254
C2	C4	0.094721210302
C3	C4	1.6485466641
C1	S5	1.2530860456
C2	S5	0.15735315867
C3	S5	0.16512806607
C4	S5	1.307084824
C1	Li6	0.0032842059483
C2	Li6	0.0018856690802
C3	Li6	0.0077867019151
C4	Li6	0.14958271546
S5	Li6	0.0074140745189
C1	H7	0.98753855186
C2	H7	0.050380745451
C3	H7	0.011009069151
C4	H7	0.018844204143
S5	H7	0.044108831879
Li6	H7	0.00045536302005
C1	H8	0.060415586332
C2	H8	0.98105890729
C3	H8	0.039595558001
C4	H8	0.01083747151
S5	H8	0.021898416639
Li6	H8	0.00028981435409
H7	H8	0.0040401711617
C1	H9	0.0099056100056
C2	H9	0.045686493278

C3	H9	0.98684490181
C4	H9	0.068591067119
S5	H9	0.024798090605
Li6	H9	0.00077302496807
H7	H9	0.0015650445175
H8	H9	0.0031062166992

### 3-BROMOTHIOPHENE

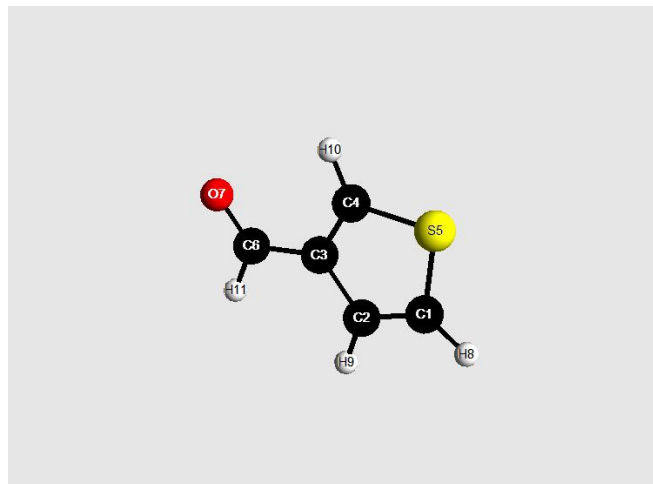


#### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6062173261
C1	C3	0.094571417482
C2	C3	1.1695797975
C1	C4	0.14052425355
C2	C4	0.079596609706
C3	C4	1.5916387945
C1	S5	1.2563218158
C2	S5	0.1469017919
C3	S5	0.15174706502
C4	S5	1.2460227376
C1	Br6	0.015628239494
C2	Br6	0.070478613366
C3	Br6	1.1398402451
C4	Br6	0.10466649019
S5	Br6	0.037435515748
C1	H7	0.97486296348
C2	H7	0.046858145699
C3	H7	0.009685190011
C4	H7	0.013733669567
S5	H7	0.043239302363
Br6	H7	0.0024466338544
C1	H8	0.053509515156
C2	H8	0.96521616675
C3	H8	0.038260001327
C4	H8	0.0075794022894
S5	H8	0.018558702388
Br6	H8	0.013843949038
H7	H8	0.0038084551036
C1	H9	0.013328304009
C2	H9	0.0086714369393

C3	H9	0.047372432944
C4	H9	0.96690087618
S5	H9	0.040277248647
Br6	H9	0.014111676709
H7	H9	0.0017943069444
H8	H9	0.0013283043771

### 3-THIOPHENECARBALDEHYDE



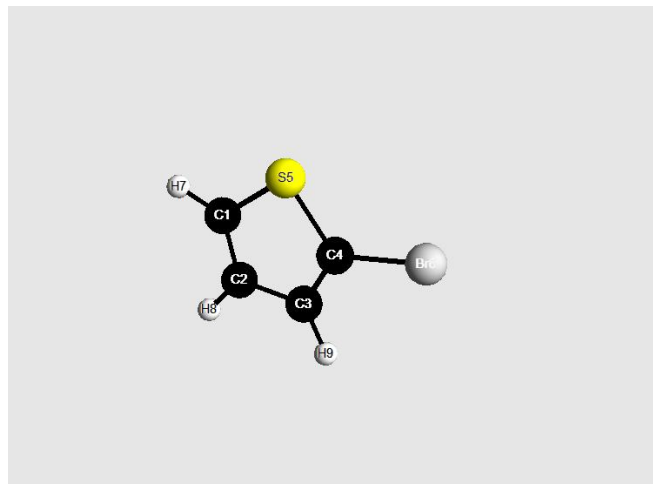
#### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6103783416
C1	C3	0.08910084054
C2	C3	1.1727044021
C1	C4	0.13935942619
C2	C4	0.08774670476
C3	C4	1.5283812926
C1	S5	1.2466003317
C2	S5	0.14435953887
C3	S5	0.14482762538
C4	S5	1.2987803759
C1	C6	0.0088386776871
C2	C6	0.043740617983
C3	C6	0.98576943897
C4	C6	0.063281509593
S5	C6	0.02190404001
C1	O7	0.0052289691511
C2	O7	0.016676252403
C3	O7	0.12706007587
C4	O7	0.053777586689
S5	O7	0.013438916837
C6	O7	1.2979029885
C1	H8	0.97725730565
C2	H8	0.047305498741
C3	H8	0.0096914610203
C4	H8	0.013459845612
S5	H8	0.043405170837
C6	H8	0.0011330381343
O7	H8	0.00086258273637
C1	H9	0.05615251018
C2	H9	0.97064225342



C3	H9	0.037401523263
C4	H9	0.0085139473301
S5	H9	0.019033733382
C6	H9	0.0050797463627
O7	H9	0.0014619172962
H8	H9	0.0038673161458
C1	C1	0.012858324594
C2	C1	0.0090978361197
C3	C1	0.04005147764
C4	C1	0.95762770057
S5	C1	0.041235806713
C6	C1	0.003774867871
O7	C1	0.014259161301
H8	C1	0.0017027416834
H9	C1	0.0013803947508
C1	H11	0.00091805533209
C2	H11	0.0083457299315
C3	H11	0.049345513189
C4	H11	0.0070494214597
S5	H11	0.003125166709
C6	H11	0.88792440389
O7	H11	0.12122393997
H8	H11	2.8388057197e-05
H9	H11	0.0057803256968
C1	H11	0.0005868699909

## 2-BROMOTHIOPHENE



### HARTREE-FOCK

Atom A	Atom B	Delocalization index
C1	C2	1.6149735592
C1	C3	0.087147991976
C2	C3	1.1721379587
C1	C4	0.13954163082
C2	C4	0.092252493157
C3	C4	1.5792413602
C1	S5	1.2404732502
C2	S5	0.14664808548
C3	S5	0.14059239104
C4	S5	1.2322908875
C1	Br6	0.027851032402
C2	Br6	0.017997725015
C3	Br6	0.093615692598
C4	Br6	1.1752830848
S5	Br6	0.096420579626
C1	H7	0.97631019661
C2	H7	0.047093707037
C3	H7	0.0095906328819
C4	H7	0.013326825714
S5	H7	0.043242276663
Br6	H7	0.0037728561342
C1	H8	0.056991913111
C2	H8	0.9728739716
C3	H8	0.038022471862
C4	H8	0.0083388040681
S5	H8	0.019252246113
Br6	H8	0.0025345496624
H7	H8	0.0040182648966
C1	H9	0.0079574927128
C2	H9	0.035536337014

C3	H9	0.9645338658
C4	H9	0.057564927937
S5	H9	0.017798957894
Br6	H9	0.014715062225
H7	H9	0.0013209233572
H8	H9	0.0027007695245