Taming the fixed-node error in diffusion Monte Carlo via range separation

Supplementary information

Anthony Scemama, Emmanuel Giner, Anouar Benali, Pierre-François Loos

August 23, 2020

Contents

1 Links to the codes

- Quantum Package : `https://github.com/QuantumPackage/qp2`
- RS-DFT Plug-in : `https://github.com/eginer/qp_plugins_lct`
- QMC=Chem : `https://gitlab.com/scemama/qmcchem`

2 Gaussian-1 set calculations

2.1 Geometries

Geometries are given in Angstrom, and taken from the NIST "Computational Chemistry Comparison and Benchmark DataBase" `http://cccbdb.nist.gov/`

2.1.1 BeH

```
2
BeH  Mult: 2 symmetry: 5
Be    0.0    0.0    0.0
H    0.0    0.0    1.3426
```

2.1.2 Be

```
1
Be  Mult: 1 symmetry: 4
Be    0.0    0.0    0.0
```

2.1.3 C2H2

```
4
C2H2  Mult: 1 symmetry: 14
C    0.0    0.0    0.6013
C    0.0    0.0    -0.6013
H    0.0    0.0    1.6644
H    0.0    0.0    -1.6644
```

2.1.4 C2H4

```
6
C2H4  Mult: 1 symmetry: 16
C    0.0    0.0    0.6695
C    0.0    0.0    -0.6695
H    0.0    0.9289    1.2321
H    0.0    -0.9289    1.2321
H    0.0    0.9289    -1.2321
H    0.0    -0.9289    -1.2321
```

2.1.5 C2H6

```
8
C2H6  Mult: 1 symmetry: 18
C    0.0    0.0    0.768
C    0.0    0.0    -0.768
H    -1.0192    0.0    1.1573
H    0.5096    0.8826    1.1573
H    0.5096    -0.8826    1.1573
```

```
H    1.0192    0.0    -1.1573
H    -0.5096    -0.8826    -1.1573
H    -0.5096    0.8826    -1.1573
```

2.1.6 $CH2_{1A1}$

```
3
CH2_1A1  Mult: 1 symmetry: 8
C    0.0    0.0    0.1734
H    0.0    0.8623    -0.5202
H    0.0    -0.8623    -0.5202
```

2.1.7 $CH2_{3B1}$

```
3
CH2_3B1  Mult: 3 symmetry: 8
C    0.0    0.0    0.1027
H    0.0    1.0042    -0.3081
H    0.0    -1.0042    -0.3081
```

2.1.8 CH3Cl

```
5
CH3Cl  Mult: 1 symmetry: 26
C    0.0    0.0    0.0
Cl    0.0    0.0    1.781
H    1.0424    0.0    -0.3901
H    -0.5212    0.9027    -0.3901
H    -0.5212    -0.9027    -0.3901
```

2.1.9 CH3

```
4
CH3  Mult: 2 symmetry: 9
C    0.0    0.0    0.0
H    1.079    0.0    0.0
H    -0.5395    -0.9344    0.0
H    -0.5395    0.9344    0.0
```

2.1.10 CH4

```
5
```

```
CH4  Mult: 1 symmetry: 10
C    0.0    0.0    0.0
H    0.6276    0.6276    0.6276
H    0.6276    -0.6276    -0.6276
H    -0.6276    0.6276    -0.6276
H    -0.6276    -0.6276    0.6276
```

2.1.11 CH

```
2
CH  Mult: 2 symmetry: 7
C    0.0    0.0    0.0
H    0.0    0.0    1.1199
```

2.1.12 Cl2

```
2
Cl2  Mult: 1 symmetry: 34
Cl    0.0    0.0    0.0
Cl    0.0    0.0    1.9879
```

2.1.13 ClF

```
2
ClF  Mult: 1 symmetry: 26
Cl    0.0    0.0    1.6283
F    0.0    0.0    0.0
```

2.1.14 ClO

```
2
ClO  Mult: 2 symmetry: 25
Cl    0.0    0.0    1.5696
O    0.0    0.0    0.0
```

2.1.15 Cl

```
1
Cl  Mult: 2 symmetry: 17
Cl    0.0    0.0    0.0
```

2.1.16 CN

```
2
CN  Mult: 2 symmetry: 13
C    0.0    0.0    0.0
N    0.0    0.0    1.1718
```

2.1.17 CO2

```
3
CO2  Mult: 1 symmetry: 22
C    0.0    0.0    0.0
O    0.0    0.0    1.1621
O    0.0    0.0    -1.1621
```

2.1.18 CO

```
2
CO  Mult: 1 symmetry: 14
C    0.0    0.0    0.0
O    0.0    0.0    1.1282
```

2.1.19 CS

```
2
CS  Mult: 1 symmetry: 22
C    0.0    0.0    0.0
S    0.0    0.0    1.5349
```

2.1.20 C

```
1
C  Mult: 3 symmetry: 6
C    0.0    0.0    0.0
```

2.1.21 F2

```
2
F2  Mult: 1 symmetry: 18
F    0.0    0.0    0.0
F    0.0    0.0    1.4119
```

2.1.22 F

```
1
F  Mult: 2 symmetry: 9
F    0.0    0.0    0.0
```

2.1.23 H2CO

```
4
H2CO  Mult: 1 symmetry: 16
C    0.0    0.0    0.0
H    0.0    0.9429    -0.5876
H    0.0    -0.9429    -0.5876
O    0.0    0.0    1.205
```

2.1.24 H2O2

```
4
H2O2  Mult: 1 symmetry: 18
H    0.819    0.817    0.422
H    -0.819    -0.817    0.422
O    0.0    0.7375    -0.0528
O    0.0    -0.7375    -0.0528
```

2.1.25 H2O

```
3
H2O  Mult: 1 symmetry: 10
H    0.0    0.7572    -0.4692
H    0.0    -0.7572    -0.4692
O    0.0    0.0    0.1173
```

2.1.26 H2S

```
3
H2S  Mult: 1 symmetry: 18
H    0.0    0.9569    0.9208
H    0.0    -0.9569    0.9208
S    0.0    0.0    0.0
```

2.1.27 H3COH

```
6
H3COH  Mult: 1 symmetry: 18
C    -0.0503    0.6685    0.0
H    -1.0807    1.0417    0.0
H    0.465    1.0417    0.8924
H    0.465    1.0417    -0.8924
H    0.8544    -1.0677    0.0
O    -0.0503    -0.7585    0.0
```

2.1.28 H3CSH

```
6
H3CSH  Mult: 1 symmetry: 26
C    -0.85    -0.0344    -0.2
H    1.4219    0.5781    0.425
H    -0.9406    0.8688    -0.8219
H    -1.4219    -0.8688    -0.6469
H    -1.2031    0.1656    0.8219
S    0.9    -0.5125    -0.1219
```

2.1.29 HCl

```
2
HCl  Mult: 1 symmetry: 18
Cl    0.0    0.0    0.0
H    0.0    0.0    1.2746
```

2.1.30 HCN

```
3
HCN  Mult: 1 symmetry: 14
C    0.0    0.0    0.0
H    0.0    0.0    1.064
N    0.0    0.0    -1.156
```

2.1.31 HCO

```
3
HCO  Mult: 2 symmetry: 15
C    0.0    0.0    0.0
```

```
H    1.08    0.0    0.0
O    -0.5899    1.0427    0.0
```

2.1.32 HF

```
2
HF  Mult: 1 symmetry: 10
F    0.0    0.0    0.0
H    0.0    0.0    0.9168
```

2.1.33 HOCl

```
3
HOCl  Mult: 1 symmetry: 26
Cl    0.0362    -0.5927    0.0
H    -0.9048    1.3042    0.0
O    0.0362    1.0964    0.0
```

2.1.34 H

```
1
H  Mult: 2 symmetry: 1
H    0.0    0.0    0.0
```

2.1.35 Li2

```
2
Li2  Mult: 1 symmetry: 6
Li    0.0    0.0    0.0
Li    0.0    0.0    2.673
```

2.1.36 LiF

```
2
LiF  Mult: 1 symmetry: 12
F    0.0    0.0    0.0
Li    0.0    0.0    1.5639
```

2.1.37 LiH

```
2
LiH  Mult: 1 symmetry: 4
```

```
H    0.0    0.0    1.5949
Li    0.0    0.0    0.0
```

2.1.38 Li

```
1
Li  Mult: 2 symmetry: 3
Li    0.0    0.0    0.0
```

2.1.39 N2H4

```
6
N2H4  Mult: 1 symmetry: 18
H    -0.447    1.0031    0.7562
H    0.447    -1.0031    0.7562
H    0.9663    1.0031    0.0301
H    -0.9663    -1.0031    0.0301
N    0.0    0.723    -0.1123
N    0.0    -0.723    -0.1123
```

2.1.40 N2

```
2
N2  Mult: 1 symmetry: 14
N    0.0    0.0    0.5488
N    0.0    0.0    -0.5488
```

2.1.41 Na2

```
2
Na2  Mult: 1 symmetry: 22
Na    0.0    0.0    0.0
Na    0.0    0.0    3.0789
```

2.1.42 NaCl

```
2
NaCl  Mult: 1 symmetry: 28
Cl    0.0    0.0    2.3608
Na    0.0    0.0    0.0
```

2.1.43 Na

```
1
Na  Mult: 2 symmetry: 11
Na    0.0    0.0    0.0
```

2.1.44 NH2

```
3
NH2  Mult: 2 symmetry: 9
H    0.0    0.8036    0.6347
H    0.0    -0.8036    0.6347
N    0.0    0.0    0.0
```

2.1.45 NH3

```
4
NH3  Mult: 1 symmetry: 10
H    0.0    -0.9377    -0.3816
H    0.8121    0.4689    -0.3816
H    -0.8121    0.4689    -0.3816
N    0.0    0.0    0.0
```

2.1.46 NH

```
2
NH  Mult: 3 symmetry: 8
H    0.0    0.0    1.0362
N    0.0    0.0    0.0
```

2.1.47 NO

```
2
NO  Mult: 2 symmetry: 15
N    0.0    0.0    1.1508
O    0.0    0.0    0.0
```

2.1.48 N

```
1
N  Mult: 4 symmetry: 7
N    0.0    0.0    0.0
```

2.1.49 O2

```
2
O2  Mult: 3 symmetry: 16
O    0.0    0.0    0.0
O    0.0    0.0    1.2075
```

2.1.50 OH

```
2
OH  Mult: 2 symmetry: 9
H    0.0    0.0    0.9697
O    0.0    0.0    0.0
```

2.1.51 O

```
1
O  Mult: 3 symmetry: 8
O    0.0    0.0    0.0
```

2.1.52 P2

```
2
P2  Mult: 1 symmetry: 30
P    0.0    0.0    0.0
P    0.0    0.0    1.8934
```

2.1.53 PH2

```
3
PH2  Mult: 2 symmetry: 17
H    0.0    1.0229    0.9964
H    0.0    -1.0229    0.9964
P    0.0    0.0    0.0
```

2.1.54 PH3

```
4
PH3  Mult: 1 symmetry: 18
H    0.0    -1.1932    -0.7717
H    1.0333    0.5966    -0.7717
H    -1.0333    0.5966    -0.7717
```

```
P    0.0    0.0    0.0
```

2.1.55 P

```
1
P  Mult: 4
P    0.0    0.0    0.0
```

2.1.56 S2

```
2
S2  Mult: 3
S    0.0    0.0    0.0
S    0.0    0.0    1.8892
```

2.1.57 Si2H6

```
8
Si2H6  Mult: 1
H    0.0    1.3865    1.6483
H    -1.2008    -0.6933    1.6483
H    1.2008    -0.6933    1.6483
H    0.0    -1.3865    -1.6483
H    -1.2008    0.6933    -1.6483
H    1.2008    0.6933    -1.6483
Si    0.0    0.0    1.16
Si    0.0    0.0    -1.16
```

2.1.58 Si2

```
2
Si2  Mult: 3
Si    0.0    0.0    0.0
Si    0.0    0.0    2.246
```

2.1.59 $SiH2_{1A1}$

```
3
SiH2_1A1  Mult: 1
H    0.0    0.0    -1.5141
H    0.0    1.5132    0.0528
Si    0.0    0.0    0.0
```

2.1.60 $SiH2_{3B1}$

```
3
SiH2_3B1  Mult: 3
H    0.0    1.273174    -0.665412
H    0.0    -1.273174    -0.665412
Si    0.0    0.0    0.095059
```

2.1.61 SiH3

```
4
SiH3  Mult: 2
H    0.0    1.3928    -0.382
H    1.2062    -0.6964    -0.382
H    -1.2062    -0.6964    -0.382
Si    0.0    0.0    0.0819
```

2.1.62 SiH4

```
5
SiH4  Mult: 1
H    0.8544    0.8544    0.8544
H    -0.8544    -0.8544    0.8544
H    -0.8544    0.8544    -0.8544
H    0.8544    -0.8544    -0.8544
Si    0.0    0.0    0.0
```

2.1.63 SiO

```
2
SiO  Mult: 1
O    0.0    0.0    1.5097
Si    0.0    0.0    0.0
```

2.1.64 Si

```
1
Si  Mult: 3
Si    0.0    0.0    0.0
```

2.1.65 SO2

```
3
SO2  Mult: 1
O    0.0    1.2371    0.7215
O    0.0    -1.2371    0.7215
S    0.0    0.0    0.0
```

2.1.66 SO

```
2
SO  Mult: 3
O    0.0    0.0    1.4811
S    0.0    0.0    0.0
```

2.1.67 S

```
1
S  Mult: 3
S    0.0    0.0    0.0

for i in ~/G2/XYZ/*.xyz
do
    printf "*** $(basename $i)\n#+begin_example\n$(cat $i)\n#+end_example\n\n"
done
```

2.2 Basis sets

Taken from `http://www.burkatzki.com/pseudos/index.2.html`

2.2.1 VDZ-BFD

1. H

```
HYDROGEN
S 9
  1 0.013000      0.000706
  2 0.029900      -0.002119
  3 0.068770      0.057693
  4 0.158170      0.230695
  5 0.363792      0.277612
  6 0.836721      0.169833
```

```
  7 1.924458      0.097443
  8 4.426254      0.029966
  9 10.180385      -0.000452
S 1
  1 0.170483      1.000000
P 9
  1 0.003000      0.001242
  2 0.007800      -0.000913
  3 0.020281      -0.000054
  4 0.052730      -0.000238
  5 0.137097      -0.011530
  6 0.356451      -0.018235
  7 0.926774      -0.013929
  8 2.409612      -0.009395
  9 6.264991      -0.000347
```

2. Li

```
LITHIUM
S 9
  1 0.010125      0.007841
  2 0.023437      0.258118
  3 0.054251      0.423307
  4 0.125581      0.167825
  5 0.290697      -0.068332
  6 0.672909      -0.119269
  7 1.557659      0.007736
  8 3.605689      0.003630
  9 8.346494      -0.000646
S 1
  1 0.103721      1.000000
P 9
  1 0.018300      -0.005906
  2 0.031699      -0.031422
  3 0.054908      -0.043628
  4 0.095111      -0.016781
  5 0.164751      -0.078594
  6 0.285379      0.015562
  7 0.494330      -0.030830
  8 0.856273      0.006185
```

```
  9 1.483225      -0.008621
P 1
  1 0.070391      1.000000
D 1
  1 0.110720      1.000000
```

3. Be

```
BERYLLIUM
S 9
  1 0.030068      0.025105
  2 0.054002      0.178890
  3 0.096986      0.263939
  4 0.174186      0.435946
  5 0.312836      -0.008188
  6 0.561850      0.049509
  7 1.009077     -0.114576
  8 1.812290      -0.067207
  9 3.254852      0.017250
S 1
  1 0.239392      1.000000
P 9
  1 0.015064      0.735052
  2 0.028584      -0.476214
  3 0.054236      0.564806
  4 0.102911      -0.108575
  5 0.195269      0.233862
  6 0.370513      -0.009003
  7 0.703030      0.067510
  8 1.333967      -0.002868
  9 2.531139      0.017869
P 1
  1 0.222969      1.000000
D 1
  1 0.217340      1.000000
```

4. C

```
CARBON
S 9
```

```
  1 0.051344      0.013991
  2 0.102619      0.169852
  3 0.205100      0.397529
  4 0.409924      0.380369
  5 0.819297      0.180113
  6 1.637494      -0.033512
  7 3.272791      -0.121499
  8 6.541187      0.015176
  9 13.073594      -0.000705
S 1
  1 0.127852      1.000000
P 9
  1 0.029281      0.001787
  2 0.058547      0.050426
  3 0.117063      0.191634
  4 0.234064      0.302667
  5 0.468003      0.289868
  6 0.935757      0.210979
  7 1.871016      0.112024
  8 3.741035      0.054425
  9 7.480076      0.021931
P 1
  1 0.149161      1.000000
D 1
  1 0.561160      1.000000
```

5. N

```
NITROGEN
S 9
  1 0.098869      0.067266
  2 0.211443      0.334290
  3 0.452197      0.454257
  4 0.967080      0.267861
  5 2.068221      0.000248
  6 4.423150      -0.132606
  7 9.459462      0.014437
  8 20.230246      0.000359
  9 43.264919      -0.000094
S 1
```

```
  1 0.175123      1.000000
P 9
  1 0.073234      0.035758
  2 0.145867      0.153945
  3 0.290535      0.277656
  4 0.578683      0.297676
  5 1.152612      0.234403
  6 2.295756      0.140321
  7 4.572652      0.067219
  8 9.107739      0.031594
  9 18.140657      0.003301
P 1
  1 0.223042      1.000000
D 1
  1 0.832058      1.000000
```

6. O

```
OXYGEN
S 9
  1 0.125346      0.055741
  2 0.268022      0.304848
  3 0.573098      0.453752
  4 1.225429      0.295926
  5 2.620277      0.019567
  6 5.602818      -0.128627
  7 11.980245      0.012024
  8 25.616801      0.000407
  9 54.775216      -0.000076
S 1
  1 0.258551      1.000000
P 9
  1 0.083598      0.044958
  2 0.167017      0.150175
  3 0.333673      0.255999
  4 0.666627      0.281879
  5 1.331816      0.242835
  6 2.660761      0.161134
  7 5.315785      0.082308
  8 10.620108      0.039899
```

```
  9 21.217318      0.004679
P 1
  1 0.267865      1.000000
D 1
  1 1.232753      1.000000
```

7. F

```
FLUORINE
S 9
  1 0.172723      0.070240
  2 0.364875      0.311088
  3 0.770795      0.444675
  4 1.628295      0.287011
  5 3.439757      0.018759
  6 7.266451      -0.128608
  7 15.350300      0.009104
  8 32.427348      0.000810
  9 68.502433      -0.000133
S 1
  1 0.344569      1.000000
P 9
  1 0.101001      0.035321
  2 0.204414      0.136924
  3 0.413707      0.249353
  4 0.837289      0.286620
  5 1.694565      0.254541
  6 3.429580      0.169572
  7 6.941026      0.088542
  8 14.047737      0.039843
  9 28.430799      0.003378
P 1
  1 0.364831      1.000000
D 1
  1 1.722479      1.000000
```

8. Na

```
SODIUM
S 9
```

```
  1 0.013061      0.200118
  2 0.030041      0.467652
  3 0.069092      0.227738
  4 0.158908      -0.061581
  5 0.365481      -0.137533
  6 0.840589      0.003323
  7 1.933315      0.003741
  8 4.446533      -0.001117
  9 10.226816      0.000244
S 1
  1 0.865135      1.000000
P 9
  1 0.002593      -0.002840
  2 0.006741      0.005340
  3 0.017525      -0.025936
  4 0.045563      -0.053466
  5 0.118461      -0.053691
  6 0.307987      0.014439
  7 0.800738      0.006199
  8 2.081847      -0.001026
  9 5.412617      0.000168
P 1
  1 0.106025      1.000000
D 1
  1 0.050790      1.000000
```

9. Si

```
SILICON
S 9
  1 0.059887      0.167492
  2 0.130108      0.532550
  3 0.282668      0.464290
  4 0.614115      -0.002322
  5 1.334205      -0.268234
  6 2.898645      0.031921
  7 6.297493      -0.000106
  8 13.681707      -0.000145
  9 29.724387      0.000067
S 1
```

```
  1 0.059803      1.000000
P 9
  1 0.036525      0.078761
  2 0.076137      0.308331
  3 0.158712      0.417773
  4 0.330843      0.281676
  5 0.689658      0.069876
  6 1.437625      -0.056306
  7 2.996797      0.000744
  8 6.246966      -0.000259
  9 13.022097      -0.000022
P 1
  1 0.081570      1.000000
D 1
  1 0.283626      1.000000
```

10. P

```
PHOSPHORUS
S 9
  1 0.074718      0.140225
  2 0.160834      0.506746
  3 0.346202      0.499893
  4 0.745215      0.037301
  5 1.604109      -0.284591
  6 3.452917      0.024766
  7 7.432561      0.001798
  8 15.998924      -0.000314
  9 34.438408      0.000088
S 1
  1 0.077260      1.000000
P 9
  1 0.050242      0.072095
  2 0.102391      0.278735
  3 0.208669      0.411034
  4 0.425256      0.304724
  5 0.866651      0.091727
  6 1.766191      -0.057060
  7 3.599410      -0.005103
  8 7.335418      0.000328
```

```
  9 14.949217      -0.000046
P 1
  1 0.113433      1.000000
D 1
  1 0.390944      1.000000
```

11. S

```
SULFUR
S 9
  1 0.095120      0.140074
  2 0.202385      0.490942
  3 0.430611      0.515297
  4 0.916203      0.050320
  5 1.949388      -0.298908
  6 4.147674      0.019827
  7 8.824926      0.007266
  8 18.776623      -0.001602
  9 39.950656      0.000271
S 1
  1 0.098454      1.000000
P 9
  1 0.057087      0.081938
  2 0.115901      0.251826
  3 0.235305      0.376344
  4 0.477723      0.320902
  5 0.969889      0.143779
  6 1.969099      -0.045543
  7 3.997726      -0.017191
  8 8.116307      0.002580
  9 16.477979      -0.000222
P 1
  1 0.128926      1.000000
D 1
  1 0.514135      1.000000
```

12. Cl

```
CHLORINE
S 9
```

```
  1 0.119944      0.148917
  2 0.257348      0.503616
  3 0.552157      0.523995
  4 1.184691      0.013612
  5 2.541836      -0.328846
  6 5.453681      0.056309
  7 11.701243      -0.001301
  8 25.105812      -0.000294
  9 53.866226      0.000076
S 1
  1 0.120667      1.000000
P 9
  1 0.074374      0.084925
  2 0.155084      0.270658
  3 0.323378      0.396022
  4 0.674303      0.324325
  5 1.406043      0.100661
  6 2.931855      -0.069802
  7 6.113450      -0.000951
  8 12.747651      0.001501
  9 26.581165      -0.000249
P 1
  1 0.168333      1.000000
D 1
  1 0.651071      1.000000
```

2.2.2 VTZ-BFD

1. H

```
HYDROGEN
S 9
  1 0.013000      0.000706
  2 0.029900      -0.002119
  3 0.068770      0.057693
  4 0.158170      0.230695
  5 0.363792      0.277612
  6 0.836721      0.169833
  7 1.924458      0.097443
  8 4.426254      0.029966
```

```
  9 10.180385      -0.000452
S 1
  1 0.170654      1.000000
P 9
  1 0.003000      0.001242
  2 0.007800      -0.000913
  3 0.020281      -0.000054
  4 0.052730      -0.000238
  5 0.137097      -0.011530
  6 0.356451      -0.018235
  7 0.926774      -0.013929
  8 2.409612      -0.009395
  9 6.264991      -0.000347
P 1
  1 0.495357      1.000000
D 1
  1 0.955745      1.000000
```

2. Li

```
LITHIUM
S 9
  1 0.010125      0.007841
  2 0.023437      0.258118
  3 0.054251      0.423307
  4 0.125581      0.167825
  5 0.290697      -0.068332
  6 0.672909      -0.119269
  7 1.557659      0.007736
  8 3.605689      0.003630
  9 8.346494      -0.000646
S 1
  1 0.026170      1.000000
S 1
  1 0.132259      1.000000
P 9
  1 0.018300      -0.005906
  2 0.031699      -0.031422
  3 0.054908      -0.043628
```

```
  4 0.095111      -0.016781
  5 0.164751      -0.078594
  6 0.285379      0.015562
  7 0.494330      -0.030830
  8 0.856273      0.006185
  9 1.483225      -0.008621
P 1
  1 0.052959      1.000000
P 1
  1 0.110075      1.000000
D 1
  1 0.067795      1.000000
D 1
  1 0.177140      1.000000
F 1
  1 0.180758      1.000000
```

3. Be

```
BERYLLIUM
S 9
  1 0.030068      0.025105
  2 0.054002      0.178890
  3 0.096986      0.263939
  4 0.174186      0.435946
  5 0.312836      -0.008188
  6 0.561850      0.049509
  7 1.009077     -0.114576
  8 1.812290      -0.067207
  9 3.254852      0.017250
S 1
  1 0.060913      1.000000
S 1
  1 0.357735      1.000000
P 9
  1 0.015064      0.735052
  2 0.028584      -0.476214
  3 0.054236      0.564806
  4 0.102911      -0.108575
```

```
  5 0.195269      0.233862
  6 0.370513      -0.009003
  7 0.703030      0.067510
  8 1.333967      -0.002868
  9 2.531139      0.017869
P 1
  1 0.728274      1.000000
P 1
  1 0.165173      1.000000
D 1
  1 0.113241      1.000000
D 1
  1 0.305198      1.000000
F 1
  1 0.272841      1.000000
```

4. C

```
CARBON
S 9
  1 0.051344      0.013991
  2 0.102619      0.169852
  3 0.205100      0.397529
  4 0.409924      0.380369
  5 0.819297      0.180113
  6 1.637494      -0.033512
  7 3.272791      -0.121499
  8 6.541187      0.015176
  9 13.073594      -0.000705
S 1
  1 0.921552      1.000000
S 1
  1 0.132800      1.000000
P 9
  1 0.029281      0.001787
  2 0.058547      0.050426
  3 0.117063      0.191634
  4 0.234064      0.302667
  5 0.468003      0.289868
```

```
  6 0.935757      0.210979
  7 1.871016      0.112024
  8 3.741035      0.054425
  9 7.480076      0.021931
P 1
  1 0.126772      1.000000
P 1
  1 0.376742      1.000000
D 1
  1 0.329486      1.000000
D 1
  1 1.141611      1.000000
F 1
  1 0.773485      1.000000
```

5. N

```
NITROGEN
S 9
  1 0.098869      0.067266
  2 0.211443      0.334290
  3 0.452197      0.454257
  4 0.967080      0.267861
  5 2.068221      0.000248
  6 4.423150      -0.132606
  7 9.459462      0.014437
  8 20.230246      0.000359
  9 43.264919      -0.000094
S 1
  1 1.202183      1.000000
S 1
  1 0.163243      1.000000
P 9
  1 0.073234      0.035758
  2 0.145867      0.153945
  3 0.290535      0.277656
  4 0.578683      0.297676
  5 1.152612      0.234403
  6 2.295756      0.140321
```

```
  7 4.572652      0.067219
  8 9.107739      0.031594
  9 18.140657      0.003301
P 1
  1 0.170104      1.000000
P 1
  1 0.517547      1.000000
D 1
  1 0.483567      1.000000
D 1
  1 1.712416      1.000000
F 1
  1 1.093097      1.000000
```

6. O

```
OXYGEN
S 9
  1 0.125346      0.055741
  2 0.268022      0.304848
  3 0.573098      0.453752
  4 1.225429      0.295926
  5 2.620277      0.019567
  6 5.602818      -0.128627
  7 11.980245      0.012024
  8 25.616801      0.000407
  9 54.775216      -0.000076
S 1
  1 1.686633      1.000000
S 1
  1 0.237997      1.000000
P 9
  1 0.083598      0.044958
  2 0.167017      0.150175
  3 0.333673      0.255999
  4 0.666627      0.281879
  5 1.331816      0.242835
  6 2.660761      0.161134
  7 5.315785      0.082308
```

```
  8 10.620108      0.039899
  9 21.217318      0.004679
P 1
  1 0.184696      1.000000
P 1
  1 0.600621      1.000000
D 1
  1 0.669340      1.000000
D 1
  1 2.404278      1.000000
F 1
  1 1.423104      1.000000
```

7. F

```
FLUORINE
S 9
  1 0.172723      0.070240
  2 0.364875      0.311088
  3 0.770795      0.444675
  4 1.628295      0.287011
  5 3.439757      0.018759
  6 7.266451      -0.128608
  7 15.350300      0.009104
  8 32.427348      0.000810
  9 68.502433      -0.000133
S 1
  1 2.289795      1.000000
S 1
  1 0.327712      1.000000
P 9
  1 0.101001      0.035321
  2 0.204414      0.136924
  3 0.413707      0.249353
  4 0.837289      0.286620
  5 1.694565      0.254541
  6 3.429580      0.169572
  7 6.941026      0.088542
  8 14.047737      0.039843
```

```
  9 28.430799      0.003378
P 1
  1 0.243660      1.000000
P 1
  1 0.804181      1.000000
D 1
  1 0.900763      1.000000
D 1
  1 3.297425      1.000000
F 1
  1 1.859274      1.000000
```

8. Na

```
SODIUM
S 9
  1 0.013061      0.200118
  2 0.030041      0.467652
  3 0.069092      0.227738
  4 0.158908      -0.061581
  5 0.365481      -0.137533
  6 0.840589      0.003323
  7 1.933315      0.003741
  8 4.446533      -0.001117
  9 10.226816      0.000244
S 1
  1 0.067854      1.000000
S 1
  1 0.550451      1.000000
P 9
  1 0.002593      -0.002840
  2 0.006741      0.005340
  3 0.017525      -0.025936
  4 0.045563      -0.053466
  5 0.118461      -0.053691
  6 0.307987      0.014439
  7 0.800738      0.006199
  8 2.081847      -0.001026
  9 5.412617      0.000168
```

```
P 1
  1 0.089406      1.000000
P 1
  1 0.619273      1.000000
D 1
  1 0.086920      1.000000
D 1
  1 0.693014      1.000000
F 1
  1 0.132402      1.000000
```

9. Si

```
SILICON
S 9
  1 0.059887      0.167492
  2 0.130108      0.532550
  3 0.282668      0.464290
  4 0.614115      -0.002322
  5 1.334205      -0.268234
  6 2.898645      0.031921
  7 6.297493      -0.000106
  8 13.681707      -0.000145
  9 29.724387      0.000067
S 1
  1 0.090113      1.000000
S 1
  1 0.507467      1.000000
P 9
  1 0.036525      0.078761
  2 0.076137      0.308331
  3 0.158712      0.417773
  4 0.330843      0.281676
  5 0.689658      0.069876
  6 1.437625      -0.056306
  7 2.996797      0.000744
  8 6.246966      -0.000259
  9 13.022097      -0.000022
P 1
```

```
  1 0.056148      1.000000
P 1
  1 0.146758      1.000000
D 1
  1 0.170395      1.000000
D 1
  1 0.539756      1.000000
F 1
  1 0.352999      1.000000
```

10. P

```
PHOSPHORUS
S 9
  1 0.074718      0.140225
  2 0.160834      0.506746
  3 0.346202      0.499893
  4 0.745215      0.037301
  5 1.604109      -0.284591
  6 3.452917      0.024766
  7 7.432561      0.001798
  8 15.998924      -0.000314
  9 34.438408      0.000088
S 1
  1 0.115288      1.000000
S 1
  1 0.646066      1.000000
P 9
  1 0.050242      0.072095
  2 0.102391      0.278735
  3 0.208669      0.411034
  4 0.425256      0.304724
  5 0.866651      0.091727
  6 1.766191      -0.057060
  7 3.599410      -0.005103
  8 7.335418      0.000328
  9 14.949217      -0.000046
P 1
  1 0.076568      1.000000
```

```
P 1
  1 0.200301      1.000000
D 1
  1 0.234543      1.000000
D 1
  1 0.753299      1.000000
F 1
  1 0.468762      1.000000
```

11. S

```
SULFUR
S 9
  1 0.095120      0.140074
  2 0.202385      0.490942
  3 0.430611      0.515297
  4 0.916203      0.050320
  5 1.949388      -0.298908
  6 4.147674      0.019827
  7 8.824926      0.007266
  8 18.776623      -0.001602
  9 39.950656      0.000271
S 1
  1 0.146642      1.000000
S 1
  1 0.792025      1.000000
P 9
  1 0.057087      0.081938
  2 0.115901      0.251826
  3 0.235305      0.376344
  4 0.477723      0.320902
  5 0.969889      0.143779
  6 1.969099      -0.045543
  7 3.997726      -0.017191
  8 8.116307      0.002580
  9 16.477979      -0.000222
P 1
  1 0.088694      1.000000
P 1
```

```
  1 0.247967      1.000000
D 1
  1 0.292889      1.000000
D 1
  1 0.950659      1.000000
F 1
  1 0.573218      1.000000
```

12. Cl

```
CHLORINE
S 9
  1 0.119944      0.148917
  2 0.257348      0.503616
  3 0.552157      0.523995
  4 1.184691      0.013612
  5 2.541836      -0.328846
  6 5.453681      0.056309
  7 11.701243      -0.001301
  8 25.105812      -0.000294
  9 53.866226      0.000076
S 1
  1 0.185613      1.000000
S 1
  1 0.991560      1.000000
P 9
  1 0.074374      0.084925
  2 0.155084      0.270658
  3 0.323378      0.396022
  4 0.674303      0.324325
  5 1.406043      0.100661
  6 2.931855      -0.069802
  7 6.113450      -0.000951
  8 12.747651      0.001501
  9 26.581165      -0.000249
P 1
  1 0.112268      1.000000
P 1
  1 0.309583      1.000000
```

```
D 1
  1 0.352357      1.000000
D 1
  1 1.128796      1.000000
F 1
  1 0.731999      1.000000
```

2.2.3 VQZ-BFD

1. H

```
HYDROGEN
S 9
  1 0.013000      0.000706
  2 0.029900      -0.002119
  3 0.068770      0.057693
  4 0.158170      0.230695
  5 0.363792      0.277612
  6 0.836721      0.169833
  7 1.924458      0.097443
  8 4.426254      0.029966
  9 10.180385      -0.000452
S 1
  1 0.120599      1.000000
S 1
  1 0.404783      1.000000
S 1
  1 0.715129      1.000000
P 9
  1 0.003000      0.001242
  2 0.007800      -0.000913
  3 0.020281      -0.000054
  4 0.052730      -0.000238
  5 0.137097      -0.011530
  6 0.356451      -0.018235
  7 0.926774      -0.013929
  8 2.409612      -0.009395
  9 6.264991      -0.000347
P 1
  1 0.774536      1.000000
```

```
P 1
  1 0.263038      1.000000
D 1
  1 2.315883      1.000000
D 1
  1 0.636656      1.000000
F 1
  1 1.130819      1.000000
```

2. Li

```
LITHIUM
S 9
  1 0.010125      0.007841
  2 0.023437      0.258118
  3 0.054251      0.423307
  4 0.125581      0.167825
  5 0.290697      -0.068332
  6 0.672909      -0.119269
  7 1.557659      0.007736
  8 3.605689      0.003630
  9 8.346494      -0.000646
S 1
  1 0.024834      1.000000
S 1
  1 0.109770      1.000000
S 1
  1 0.519693      1.000000
P 9
  1 0.018300      -0.005906
  2 0.031699      -0.031422
  3 0.054908      -0.043628
  4 0.095111      -0.016781
  5 0.164751      -0.078594
  6 0.285379      0.015562
  7 0.494330      -0.030830
  8 0.856273      0.006185
  9 1.483225      -0.008621
P 1
```

```
  1 0.070662      1.000000
P 1
  1 0.115823      1.000000
P 1
  1 0.207505      1.000000
D 1
  1 0.029817      1.000000
D 1
  1 0.089353      1.000000
D 1
  1 0.214990      1.000000
F 1
  1 0.099930      1.000000
F 1
  1 0.240323      1.000000
G 1
  1 0.199570      1.000000
```

3. Be

```
BERYLLIUM
S 9
  1 0.030068      0.025105
  2 0.054002      0.178890
  3 0.096986      0.263939
  4 0.174186      0.435946
  5 0.312836      -0.008188
  6 0.561850      0.049509
  7 1.009077     -0.114576
  8 1.812290      -0.067207
  9 3.254852      0.017250
S 1
  1 0.012287      1.000000
S 1
  1 0.175341      1.000000
S 1
  1 1.244398      1.000000
P 9
  1 0.015064      0.735052
```

```
  2 0.028584      -0.476214
  3 0.054236      0.564806
  4 0.102911      -0.108575
  5 0.195269      0.233862
  6 0.370513      -0.009003
  7 0.703030      0.067510
  8 1.333967      -0.002868
  9 2.531139      0.017869
P 1
  1 0.317061      1.000000
P 1
  1 1.585739      1.000000
P 1
  1 0.108346      1.000000
D 1
  1 0.125228      1.000000
D 1
  1 0.801065      1.000000
D 1
  1 0.301656      1.000000
F 1
  1 0.153439      1.000000
F 1
  1 0.377536      1.000000
G 1
  1 0.338801      1.000000
```

4. C

```
CARBON
S 9
  1 0.051344      0.013991
  2 0.102619      0.169852
  3 0.205100      0.397529
  4 0.409924      0.380369
  5 0.819297      0.180113
  6 1.637494      -0.033512
  7 3.272791      -0.121499
  8 6.541187      0.015176
```

```
  9 13.073594      -0.000705
S 1
  1 0.109576      1.000000
S 1
  1 0.846879      1.000000
S 1
  1 0.269659      1.000000
P 9
  1 0.029281      0.001787
  2 0.058547      0.050426
  3 0.117063      0.191634
  4 0.234064      0.302667
  5 0.468003      0.289868
  6 0.935757      0.210979
  7 1.871016      0.112024
  8 3.741035      0.054425
  9 7.480076      0.021931
P 1
  1 0.105389      1.000000
P 1
  1 0.313254      1.000000
P 1
  1 0.804681      1.000000
D 1
  1 0.240171      1.000000
D 1
  1 0.684884      1.000000
D 1
  1 2.013760      1.000000
F 1
  1 0.457302      1.000000
F 1
  1 1.324930      1.000000
G 1
  1 1.034180      1.000000
```

5. N

```
NITROGEN
```

```
S 9
  1 0.098869      0.067266
  2 0.211443      0.334290
  3 0.452197      0.454257
  4 0.967080      0.267861
  5 2.068221      0.000248
  6 4.423150      -0.132606
  7 9.459462      0.014437
  8 20.230246      0.000359
  9 43.264919      -0.000094
S 1
  1 0.135764      1.000000
S 1
  1 0.310826      1.000000
S 1
  1 1.625001      1.000000
P 9
  1 0.073234      0.035758
  2 0.145867      0.153945
  3 0.290535      0.277656
  4 0.578683      0.297676
  5 1.152612      0.234403
  6 2.295756      0.140321
  7 4.572652      0.067219
  8 9.107739      0.031594
  9 18.140657      0.003301
P 1
  1 0.140736      1.000000
P 1
  1 0.413103      1.000000
P 1
  1 1.020750      1.000000
D 1
  1 0.346233      1.000000
D 1
  1 1.009895      1.000000
D 1
  1 3.028459      1.000000
F 1
  1 0.691129      1.000000
```

```
F 1
  1 2.024747      1.000000
G 1
  1 1.357512      1.000000
```

6. O

```
OXYGEN
S 9
  1 0.125346      0.055741
  2 0.268022      0.304848
  3 0.573098      0.453752
  4 1.225429      0.295926
  5 2.620277      0.019567
  6 5.602818      -0.128627
  7 11.980245      0.012024
  8 25.616801      0.000407
  9 54.775216      -0.000076
S 1
  1 0.224380      1.000000
S 1
  1 0.843157      1.000000
S 1
  1 1.351771      1.000000
P 9
  1 0.083598      0.044958
  2 0.167017      0.150175
  3 0.333673      0.255999
  4 0.666627      0.281879
  5 1.331816      0.242835
  6 2.660761      0.161134
  7 5.315785      0.082308
  8 10.620108      0.039899
  9 21.217318      0.004679
P 1
  1 0.148562      1.000000
P 1
  1 0.452364      1.000000
P 1
```

```
  1 1.106737      1.000000
D 1
  1 0.455711      1.000000
D 1
  1 1.344331      1.000000
D 1
  1 4.008867      1.000000
F 1
  1 0.876289      1.000000
F 1
  1 2.763115      1.000000
G 1
  1 1.759081      1.000000
```

7. F

```
FLUORINE
S 9
  1 0.172723      0.070240
  2 0.364875      0.311088
  3 0.770795      0.444675
  4 1.628295      0.287011
  5 3.439757      0.018759
  6 7.266451      -0.128608
  7 15.350300      0.009104
  8 32.427348      0.000810
  9 68.502433      -0.000133
S 1
  1 0.294345      1.000000
S 1
  1 1.048013      1.000000
S 1
  1 1.705653      1.000000
P 9
  1 0.101001      0.035321
  2 0.204414      0.136924
  3 0.413707      0.249353
  4 0.837289      0.286620
  5 1.694565      0.254541
```

```
  6 3.429580      0.169572
  7 6.941026      0.088542
  8 14.047737      0.039843
  9 28.430799      0.003378
P 1
  1 0.205806      1.000000
P 1
  1 0.647240      1.000000
P 1
  1 1.650688      1.000000
D 1
  1 0.587354      1.000000
D 1
  1 1.724392      1.000000
D 1
  1 4.998085      1.000000
F 1
  1 1.178147      1.000000
F 1
  1 3.694285      1.000000
G 1
  1 2.406583      1.000000
```

8. Na

```
SODIUM
S 9
  1 0.013061      0.200118
  2 0.030041      0.467652
  3 0.069092      0.227738
  4 0.158908      -0.061581
  5 0.365481      -0.137533
  6 0.840589      0.003323
  7 1.933315      0.003741
  8 4.446533      -0.001117
  9 10.226816      0.000244
S 1
  1 0.064915      1.000000
S 1
```

```
  1 1.134458      1.000000
S 1
  1 0.771046      1.000000
P 9
  1 0.002593      -0.002840
  2 0.006741      0.005340
  3 0.017525      -0.025936
  4 0.045563      -0.053466
  5 0.118461      -0.053691
  6 0.307987      0.014439
  7 0.800738      0.006199
  8 2.081847      -0.001026
  9 5.412617      0.000168
P 1
  1 0.059662      1.000000
P 1
  1 0.096714      1.000000
P 1
  1 0.552976      1.000000
D 1
  1 0.046917      1.000000
D 1
  1 0.813868      1.000000
D 1
  1 0.127780      1.000000
F 1
  1 0.129992      1.000000
F 1
  1 0.626429      1.000000
G 1
  1 0.588778      1.000000
```

9. Si

```
SILICON
S 9
  1 0.059887      0.167492
  2 0.130108      0.532550
  3 0.282668      0.464290
```

```
  4 0.614115      -0.002322
  5 1.334205      -0.268234
  6 2.898645      0.031921
  7 6.297493      -0.000106
  8 13.681707      -0.000145
  9 29.724387      0.000067
S 1
  1 0.079900      1.000000
S 1
  1 0.206024      1.000000
S 1
  1 0.435017      1.000000
P 9
  1 0.036525      0.078761
  2 0.076137      0.308331
  3 0.158712      0.417773
  4 0.330843      0.281676
  5 0.689658      0.069876
  6 1.437625      -0.056306
  7 2.996797      0.000744
  8 6.246966      -0.000259
  9 13.022097      -0.000022
P 1
  1 0.054575      1.000000
P 1
  1 0.599112      1.000000
P 1
  1 0.134681      1.000000
D 1
  1 0.133118      1.000000
D 1
  1 0.350967      1.000000
D 1
  1 1.063961      1.000000
F 1
  1 0.211319      1.000000
F 1
  1 0.535932      1.000000
G 1
  1 0.465365      1.000000
```

10. P

```
PHOSPHORUS
S 9
  1 0.074718      0.140225
  2 0.160834      0.506746
  3 0.346202      0.499893
  4 0.745215      0.037301
  5 1.604109      -0.284591
  6 3.452917      0.024766
  7 7.432561      0.001798
  8 15.998924      -0.000314
  9 34.438408      0.000088
S 1
  1 0.098851      1.000000
S 1
  1 0.255593      1.000000
S 1
  1 0.546057      1.000000
P 9
  1 0.050242      0.072095
  2 0.102391      0.278735
  3 0.208669      0.411034
  4 0.425256      0.304724
  5 0.866651      0.091727
  6 1.766191      -0.057060
  7 3.599410      -0.005103
  8 7.335418      0.000328
  9 14.949217      -0.000046
P 1
  1 0.074522      1.000000
P 1
  1 0.764539      1.000000
P 1
  1 0.182211      1.000000
D 1
  1 0.186505      1.000000
D 1
```

```
  1 0.502400      1.000000
D 1
  1 1.576445      1.000000
F 1
  1 0.280702      1.000000
F 1
  1 0.719161      1.000000
G 1
  1 0.599144      1.000000
```

11. S

```
SULFUR
S 9
  1 0.095120      0.140074
  2 0.202385      0.490942
  3 0.430611      0.515297
  4 0.916203      0.050320
  5 1.949388      -0.298908
  6 4.147674      0.019827
  7 8.824926      0.007266
  8 18.776623      -0.001602
  9 39.950656      0.000271
S 1
  1 0.123759      1.000000
S 1
  1 0.315587      1.000000
S 1
  1 0.651905      1.000000
P 9
  1 0.057087      0.081938
  2 0.115901      0.251826
  3 0.235305      0.376344
  4 0.477723      0.320902
  5 0.969889      0.143779
  6 1.969099      -0.045543
  7 3.997726      -0.017191
  8 8.116307      0.002580
  9 16.477979      -0.000222
```

```
P 1
  1 0.078717      1.000000
P 1
  1 0.202707      1.000000
P 1
  1 0.301333      1.000000
D 1
  1 0.215701      1.000000
D 1
  1 0.560638      1.000000
D 1
  1 1.588204      1.000000
F 1
  1 0.356554      1.000000
F 1
  1 0.961826      1.000000
G 1
  1 0.694803      1.000000
```

12. Cl

```
CHLORINE
S 9
  1 0.119944      0.148917
  2 0.257348      0.503616
  3 0.552157      0.523995
  4 1.184691      0.013612
  5 2.541836      -0.328846
  6 5.453681      0.056309
  7 11.701243      -0.001301
  8 25.105812      -0.000294
  9 53.866226      0.000076
S 1
  1 0.161594      1.000000
S 1
  1 0.440111      1.000000
S 1
  1 0.848928      1.000000
P 9
```

```
  1 0.074374      0.084925
  2 0.155084      0.270658
  3 0.323378      0.396022
  4 0.674303      0.324325
  5 1.406043      0.100661
  6 2.931855      -0.069802
  7 6.113450      -0.000951
  8 12.747651      0.001501
  9 26.581165      -0.000249
P 1
  1 0.111309      1.000000
P 1
  1 1.286881      1.000000
P 1
  1 0.289403      1.000000
D 1
  1 0.253063      1.000000
D 1
  1 0.642589      1.000000
D 1
  1 1.654717      1.000000
F 1
  1 0.448175      1.000000
F 1
  1 1.189807      1.000000
G 1
  1 0.848307      1.000000
```

2.3 Pseudopotentials

Taken from `http://www.burkatzki.com/pseudos/index.2.html`

2.3.1 H

```
H GEN 0 0
3
1.00000000 1 4.47692410
4.47692410 3 2.97636451
-4.32112340 2 3.01841596
```

2.3.2 Li

```
Li GEN 2 1
3
1.00000000 1 5.41040609
5.41040609 3 2.70520138
-4.60151975 2 2.07005488
1
7.09172172 2 1.34319829
```

2.3.3 Be

```
Be GEN 2 1
3
2.00000000 1 4.58686001
9.17372003 3 2.29371778
-8.12599146 2 2.10401964
1
14.90499810 2 2.71723988
```

2.3.4 C

```
C GEN 2 1
3
4.00000000 1 8.35973821
33.43895285 3 4.48361888
-19.17537323 2 3.93831258
1
22.55164191 2 5.02991637
```

2.3.5 N

```
N GEN 2 1
3
5.00000000 1 9.23501007
46.17505034 3 7.66830008
-30.18893534 2 7.34486070
1
31.69720409 2 6.99536540
```

2.3.6 O

```
O GEN 2 1
3
6.00000000 1 9.29793903
55.78763416 3 8.86492204
-38.81978498 2 8.62925665
1
38.41914135 2 8.71924452
```

2.3.7 F

```
F GEN 2 1
3
7.00000000 1 11.39210685
79.74474797 3 10.74911370
-49.45159098 2 10.45120693
1
50.25646328 2 11.30345826
```

2.3.8 Na

```
Na GEN 10 2
3
1.00000000 1 5.35838717
5.35838717 3 3.67918975
-2.07764789 2 1.60507673
1
10.69640234 2 1.32389367
1
10.11238853 2 1.14052020
```

2.3.9 Si

```
Si GEN 10 2
3
4.00000000 1 1.80721061
7.22884246 3 9.99633089
-13.06725590 2 2.50043232
1
21.20531613 2 2.26686403
```

```
1
15.43693603 2 2.11659661
```

2.3.10 P

```
P GEN 10 2
3
5.00000000 1 2.02622810
10.13114051 3 9.95970113
-14.94375088 2 2.74841795
1
23.62479480 2 2.60470698
1
18.18547203 2 2.54957900
```

2.3.11 S

```
S GEN 10 2
3
6.00000000 1 2.42178462
14.53070769 3 6.74148698
-17.52965289 2 3.06094751
1
25.99260928 2 2.94272173
1
18.93356489 2 2.84566981
```

2.3.12 Cl

```
Cl GEN 10 2
3
7.00000000 1 2.41079533
16.87556731 3 5.29139158
-18.80917558 2 2.91105513
1
28.59107316 2 3.34528827
1
19.37583724 2 3.12408551
```

2.4 Python functions to compute MAE, MSE adn RMSE

2.5 VDZ-BFD

2.5.1 CCSD(T)

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-1.000525			
C	-5.409242			
Cl	-14.874294			
F	-24.092526			
H	-0.499045			
Li	-0.195611			
N	-9.760315			
Na	-0.174227			
O	-15.829829			
P	-6.441709			
S	-10.063896			
Si	-3.747375			
BeH	-1.553504	0.053934	0.079400	-15.979980
C2H2	-12.404798	0.588225	0.642400	-33.995396
C2H4	-13.652947	0.838283	0.899000	-38.100407
C2H6	-14.882446	1.069692	1.136900	-42.173979
CH	-6.030335	0.122048	0.133900	-7.437258
$CH2_{1A1}$	-6.673470	0.266138	0.288900	-14.283148
$CH2_{3B1}$	-6.693049	0.285717	0.304100	-11.535254
CH3	-7.368024	0.461647	0.490800	-18.293738
CH3Cl	-22.364720	0.584048	0.631000	-29.462716
CH4	-8.039741	0.634319	0.670300	-22.578590
CN	-15.416198	0.246642	0.288800	-26.454701
CO	-21.619072	0.380002	0.413700	-21.146121
CO2	-37.626356	0.557457	0.621400	-40.124644
CS	-15.713978	0.240840	0.274000	-20.808005
Cl2	-29.811893	0.063305	0.094000	-19.261488
ClF	-39.032802	0.065982	0.100100	-21.409434
ClO	-30.768878	0.064755	0.104700	-25.065634
F2	-48.218609	0.033557	0.062200	-17.973728
H2CO	-22.786343	0.549183	0.596700	-29.817652
H2O	-17.163976	0.336057	0.371900	-22.492118
H2O2	-33.026612	0.368864	0.429400	-37.986866
H2S	-11.327615	0.265628	0.292000	-16.548623
H3COH	-23.990033	0.754781	0.818700	-40.109587
H3CSH	-18.166535	0.697217	0.757000	-37.514699
HCN	-16.115311	0.446710	0.496900	-31.494849
HCO	-22.141199	0.403084	0.444700	-26.114492
HCl	-15.530195	0.156855	0.171000	-8.875933
HF	-24.793702	0.202131	0.226100	-15.040593
HOCl	-31.422422	0.219254	0.264700	-28.517956
Li2	-0.429057	0.037834	0.038900	-0.668695

2.5.2 DFT

1. PBE

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.993247			
C	-5.417931			
Cl	-14.942111			
F	-24.188803			
H	-0.497466			
Li	-0.200657			
N	-9.785099			
Na	-0.179448			
O	-15.896735			
P	-6.463474			
S	-10.111396			
Si	-3.764725			
BeH	-1.561314	0.070600	0.079400	-5.522139
C2H2	-12.471750	0.640955	0.642400	-0.906510
C2H4	-13.725004	0.899276	0.899000	0.173384
C2H6	-14.956934	1.136273	1.136900	-0.393184
CH	-6.049219	0.133822	0.133900	-0.049116
$CH2_{1A1}$	-6.693746	0.280882	0.288900	-5.031326
$CH2_{3B1}$	-6.725160	0.312297	0.304100	5.143465
CH3	-7.403645	0.493315	0.490800	1.578365
CH3Cl	-22.481075	0.628633	0.631000	-1.485142
CH4	-8.075706	0.667910	0.670300	-1.499859
CN	-15.499625	0.296596	0.288800	4.891804
CO	-21.720791	0.406126	0.413700	-4.752941
CO2	-37.836708	0.625309	0.621400	2.452746
CS	-15.798388	0.269061	0.274000	-3.099051
Cl2	-29.973609	0.089386	0.094000	-2.895432
ClF	-39.225356	0.094442	0.100100	-3.550567
ClO	-30.943200	0.104354	0.104700	-0.217225
F2	-48.441579	0.063973	0.062200	1.112590
H2CO	-22.906450	0.596851	0.596700	0.094987
H2O	-17.246569	0.354901	0.371900	-10.667006
H2O2	-33.201882	0.413480	0.429400	-9.989827
H2S	-11.389498	0.283169	0.292000	-5.541528
H3COH	-24.113873	0.809342	0.818700	-5.872374
H3CSH	-18.268976	0.749784	0.757000	-4.528211
HCN	-16.198534	0.498038	0.496900	0.713833
HCO	-22.262019	0.449887	0.444700	3.254932
HCl	-15.604804	0.165226	0.171000	-3.623105
HF	-24.897525	0.211255	0.226100	-9.315258
HOCl	-31.590694	0.254381	0.264700	-6.475113
Li2	-0.428519	0.027204	0.038900	-7.339044
LiF	-24.593998	0.204537	0.222000	-10.958023
LiH	-0.782770	0.084646	0.092430	-4.884499
N2	-19.930500	0.360302	0.364600	-2.697095
N2H4	-22.248305	0.688242	0.699600	-7.127549
NH	-10.420288	0.137723	0.133500	2.649862

2. BLYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.988064			
C	-5.410195			
Cl	-14.916694			
F	-24.189925			
H	-0.495150			
Li	-0.196349			
N	-9.770509			
Na	-0.175409			
O	-15.891656			
P	-6.435546			
S	-10.085757			
Si	-3.745381			
BeH	-1.556618	0.073404	0.079400	-3.762589
C2H2	-12.424888	0.614199	0.642400	-17.696462
C2H4	-13.670672	0.869683	0.899000	-18.396908
C2H6	-14.894114	1.102825	1.136900	-21.382711
CH	-6.039336	0.133992	0.133900	0.057494
$CH2_{1A1}$	-6.680512	0.280018	0.288900	-5.573735
$CH2_{3B1}$	-6.700676	0.300181	0.304100	-2.459253
CH3	-7.378027	0.482382	0.490800	-5.282205
CH3Cl	-22.418187	0.605849	0.631000	-15.782783
CH4	-8.046184	0.655389	0.670300	-9.356578
CN	-15.461499	0.280795	0.288800	-5.022934
CO	-21.691791	0.389940	0.413700	-14.909668
CO2	-37.783235	0.589728	0.621400	-19.874348
CS	-15.750022	0.254070	0.274000	-12.506389
Cl2	-29.911351	0.077964	0.094000	-10.062795
ClF	-39.192330	0.085712	0.100100	-9.028879
ClO	-30.902002	0.093652	0.104700	-6.932904
F2	-48.439704	0.059855	0.062200	-1.471341
H2CO	-22.868751	0.576600	0.596700	-12.612673
H2O	-17.230950	0.348993	0.371900	-14.374084
H2O2	-33.174732	0.401119	0.429400	-17.746395
H2S	-11.356030	0.279973	0.292000	-7.547210
H3COH	-24.068207	0.785756	0.818700	-20.672837
H3CSH	-18.202429	0.725877	0.757000	-19.530185
HCN	-16.157678	0.481825	0.496900	-9.459961
HCO	-22.227978	0.430977	0.444700	-8.611273
HCl	-15.573480	0.161636	0.171000	-5.876015
HF	-24.892357	0.207283	0.226100	-11.808019
HOCl	-31.545554	0.242054	0.264700	-14.210349
Li2	-0.422799	0.030101	0.038900	-5.521584
LiF	-24.592187	0.205913	0.222000	-10.094817
LiH	-0.785101	0.093602	0.092430	0.735479
N2	-19.893203	0.352186	0.364600	-7.790038
N2H4	-22.195729	0.674112	0.699600	-15.994195
NH	-10.404192	0.138533	0.133500	3.158563

3. PBE0

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.994318			
C	-5.421146			
Cl	-14.948397			
F	-24.189146			
H	-0.499431			
Li	-0.200948			
N	-9.790708			
Na	-0.179543			
O	-15.897980			
P	-6.467798			
S	-10.116079			
Si	-3.766144			
BeH	-1.563416	0.069667	0.079400	-6.107710
C2H2	-12.469009	0.627855	0.642400	-9.126831
C2H4	-13.729397	0.889383	0.899000	-6.034906
C2H6	-14.969664	1.130787	1.136900	-3.835669
CH	-6.051735	0.131158	0.133900	-1.720354
$CH2_{1A1}$	-6.697562	0.277555	0.288900	-7.119041
$CH2_{3B1}$	-6.730766	0.310759	0.304100	4.178584
CH3	-7.410762	0.491324	0.490800	0.328793
CH3Cl	-22.489249	0.621414	0.631000	-6.015040
CH4	-8.084052	0.665184	0.670300	-3.210638
CN	-15.481772	0.269918	0.288800	-11.848704
CO	-21.707474	0.388349	0.413700	-15.908271
CO2	-37.808272	0.591167	0.621400	-18.971563
CS	-15.789677	0.252453	0.274000	-13.521048
Cl2	-29.976361	0.079568	0.094000	-9.056149
ClF	-39.215130	0.077587	0.100100	-14.126921
ClO	-30.930958	0.084582	0.104700	-12.624402
F2	-48.413376	0.035084	0.062200	-17.015433
H2CO	-22.896206	0.578219	0.596700	-11.597073
H2O	-17.243034	0.346193	0.371900	-16.131389
H2O2	-33.181595	0.386774	0.429400	-26.748059
H2S	-11.394289	0.279349	0.292000	-7.938658
H3COH	-24.112980	0.796131	0.818700	-14.162344
H3CSH	-18.277123	0.742176	0.757000	-9.302473
HCN	-16.188403	0.477119	0.496900	-12.412831
HCO	-22.247789	0.429232	0.444700	-9.706149
HCl	-15.610641	0.162814	0.171000	-5.136966
HF	-24.893575	0.204998	0.226100	-13.241447
HOCl	-31.582495	0.236687	0.264700	-17.578181
Li2	-0.429515	0.027619	0.038900	-7.079069
LiF	-24.584862	0.194768	0.222000	-17.088359
LiH	-0.783495	0.083116	0.092430	-5.844810
N2	-19.915794	0.334378	0.364600	-18.964545
N2H4	-22.245726	0.666587	0.699600	-20.715792
NH	-10.422715	0.132576	0.133500	-0.579621

4. B3LYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.998136			
C	-5.431412			
Cl	-14.958096			
F	-24.222499			
H	-0.500253			
Li	-0.200391			
N	-9.799156			
Na	-0.179112			
O	-15.920208			
P	-6.464518			
S	-10.120165			
Si	-3.766224			
BeH	-1.571692	0.073303	0.079400	-3.825922
C2H2	-12.477544	0.614215	0.642400	-17.686218
C2H4	-13.739894	0.876060	0.899000	-14.395056
C2H6	-14.980872	1.116533	1.136900	-12.780420
CH	-6.065520	0.133856	0.133900	-0.027889
$CH2_{1A1}$	-6.714134	0.282217	0.288900	-4.193516
$CH2_{3B1}$	-6.735275	0.303358	0.304100	-0.465871
CH3	-7.419748	0.487578	0.490800	-2.021549
CH3Cl	-22.501275	0.611009	0.631000	-12.544429
CH4	-8.095463	0.663040	0.670300	-4.555422
CN	-15.494947	0.264379	0.288800	-15.324218
CO	-21.734424	0.382804	0.413700	-19.387516
CO2	-37.847080	0.575252	0.621400	-28.958440
CS	-15.797931	0.246354	0.274000	-17.348432
Cl2	-29.990079	0.073886	0.094000	-12.621473
ClF	-39.257406	0.076811	0.100100	-14.613891
ClO	-30.960845	0.082540	0.104700	-13.905499
F2	-48.486531	0.041533	0.062200	-12.968601
H2CO	-22.924738	0.572612	0.596700	-15.115297
H2O	-17.269507	0.348793	0.371900	-14.499605
H2O2	-33.231658	0.390736	0.429400	-24.261910
H2S	-11.402655	0.281985	0.292000	-6.284520
H3COH	-24.142533	0.789903	0.818700	-18.070330
H3CSH	-18.285654	0.733067	0.757000	-15.018499
HCN	-16.204026	0.473206	0.496900	-14.868506
HCO	-22.274671	0.422798	0.444700	-13.743833
HCl	-15.620958	0.162609	0.171000	-5.265529
HF	-24.929058	0.206307	0.226100	-12.420602
HOCl	-31.613929	0.235372	0.264700	-18.403511
Li2	-0.432168	0.031385	0.038900	-4.716027
LiF	-24.624234	0.201344	0.222000	-12.962157
LiH	-0.794310	0.093666	0.092430	0.775841
N2	-19.935745	0.337433	0.364600	-17.047592
N2H4	-22.269483	0.670161	0.699600	-18.473055
NH	-10.435276	0.135868	0.133500	1.485985

2.5.3 $\mu = 0$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.993248				7
C	-5.415027				22
Cl	-14.939960				15
F	-24.186522				15
H	-0.497463				1
Li	-0.200622				1
N	-9.781515				15
Na	-0.179437				1
O	-15.892659				30
P	-6.462474				12
S	-10.108694				19
Si	-3.762593				21
BeH	-1.558664	0.067953	0.079400	-7.183403	15
C2H2	-12.471515	0.646535	0.642400	2.594724	23
C2H4	-13.724919	0.905013	0.899000	3.773372	47
C2H6	-14.956874	1.142042	1.136900	3.226464	95
CH	-6.046757	0.134267	0.133900	0.230129	16
$CH2_{1A1}$	-6.693162	0.283209	0.288900	-3.571043	11
$CH2_{3B1}$	-6.718171	0.308218	0.304100	2.583914	35
CH3	-7.400803	0.493387	0.490800	1.623267	34
CH3Cl	-22.480882	0.633506	0.631000	1.572723	95
CH4	-8.075889	0.671010	0.670300	0.445691	47
CN	-15.495478	0.298936	0.288800	6.360200	80
CO	-21.720728	0.413042	0.413700	-0.413200	47
CO2	-37.836668	0.636322	0.621400	9.363959	99
CS	-15.798359	0.274638	0.274000	0.400572	47
Cl2	-29.973613	0.093693	0.094000	-0.192680	47
ClF	-39.225326	0.098844	0.100100	-0.788330	95
ClO	-30.939687	0.107068	0.104700	1.485702	139
F2	-48.441566	0.068522	0.062200	3.967041	23
H2CO	-22.906390	0.603778	0.596700	4.441495	95
H2O	-17.246557	0.358972	0.371900	-8.112291	23
H2O2	-33.201845	0.421601	0.429400	-4.894030	95
H2S	-11.389511	0.285891	0.292000	-3.833390	23
H3COH	-24.114466	0.816928	0.818700	-1.111846	191
H3CSH	-18.268034	0.754461	0.757000	-1.593168	191
HCN	-16.198138	0.504133	0.496900	4.538815	23
HCO	-22.259446	0.454297	0.444700	6.022308	75
HCl	-15.604297	0.166874	0.171000	-2.589052	5
HF	-24.897651	0.213666	0.226100	-7.802434	23
HOCl	-31.590525	0.260443	0.264700	-2.671322	95
Li2	-0.428509	0.027266	0.038900	-7.300224	5
LiF	-24.593060	0.205916	0.222000	-10.092758	11
LiH	-0.782437	0.084353	0.092430	-5.068356	5
N2	-19.930424	0.367394	0.364600	1.753156	23
N2H4	-22.248700	0.695818	0.699600	-2.372950	191
NH	-10.415491	0.136513	0.133500	1.890457	45

2. DMC

	Total E Hartree	Delta E Hartree			Reference Hartree	Error kcal/mol		N
Be	-0.998148	0.000092	0.000000	0.000130				
C	-5.416660	0.000115	0.000000	0.000162				
Cl	-14.941027	0.000238	0.000000	0.000337				
F	-24.188696	0.000307	0.000000	0.000434				
H	-0.500031	0.000018	0.000000	0.000026				
Li	-0.196316	0.000015	0.000000	0.000021				
N	-9.788967	0.000036	0.000000	0.000050				
Na	-0.182137	0.000024	0.000000	0.000035				
O	-15.892761	0.000165	0.000000	0.000234				
P	-6.462282	0.000147	0.000000	0.000208				
S	-10.108631	0.000180	0.000000	0.000254				
Si	-3.758637	0.000127	0.000000	0.000179				
BeH	-1.577615	0.000141	0.079436	0.000169	0.079400	0.022764	0.105989	
C2H2	-12.484315	0.000151	0.650934	0.000277	0.642400	5.355209	0.173910	
C2H4	-13.739259	0.000229	0.905816	0.000332	0.899000	4.277377	0.208402	
C2H6	-14.981071	0.000333	1.147568	0.000419	1.136900	6.694192	0.262996	
CH	-6.049268	0.000196	0.132578	0.000228	0.133900	-0.829728	0.142843	
$CH2_{1A1}$	-6.703492	0.000238	0.286770	0.000266	0.288900	-1.336311	0.167125	
$CH2_{3B1}$	-6.724996	0.000269	0.308275	0.000295	0.304100	2.619917	0.185176	
CH3	-7.412882	0.000292	0.496130	0.000318	0.490800	3.344668	0.199835	
CH3Cl	-22.489205	0.000399	0.631425	0.000482	0.631000	0.266960	0.302320	
CH4	-8.092108	0.000399	0.675326	0.000421	0.670300	3.153570	0.264435	
CN	-15.485848	0.000492	0.280221	0.000507	0.288800	-5.383274	0.317893	
CO	-21.720292	0.000637	0.410872	0.000668	0.413700	-1.774827	0.419105	
CO2	-37.821311	0.000457	0.619130	0.000576	0.621400	-1.424287	0.361548	
CS	-15.791296	0.000506	0.266005	0.000549	0.274000	-5.016926	0.344390	
Cl2	-29.970408	0.000318	0.088353	0.000573	0.094000	-3.543283	0.359273	
ClF	-39.217307	0.000473	0.087584	0.000612	0.100100	-7.853689	0.384201	
ClO	-30.922660	0.000313	0.088872	0.000426	0.104700	-9.932428	0.267499	1
F2	-48.419510	0.000441	0.042118	0.000756	0.062200	-12.601453	0.474402	
H2CO	-22.905562	0.000327	0.596081	0.000386	0.596700	-0.388687	0.242254	
H2O	-17.253644	0.000357	0.360822	0.000395	0.371900	-6.951452	0.247730	
H2O2	-33.191401	0.000427	0.405818	0.000541	0.429400	-14.797733	0.339586	
H2S	-11.395361	0.000322	0.286668	0.000370	0.292000	-3.345828	0.232243	
H3COH	-24.124994	0.000490	0.815451	0.000535	0.818700	-2.039009	0.335828	1
H3CSH	-18.280515	0.000406	0.755102	0.000465	0.757000	-1.191089	0.291560	1
HCN	-16.202168	0.000572	0.496510	0.000585	0.496900	-0.244593	0.366861	
HCO	-22.249935	0.000774	0.440484	0.000800	0.444700	-2.645570	0.501756	
HCl	-15.609712	0.000275	0.168654	0.000364	0.171000	-1.472270	0.228279	
HF	-24.906034	0.000455	0.217308	0.000549	0.226100	-5.517341	0.344784	
HOCl	-31.584385	0.000377	0.250566	0.000476	0.264700	-8.869252	0.298768	
Li2	-0.427876	0.000084	0.035245	0.000089	0.038900	-2.293696	0.055644	
LiF	-24.603768	0.000419	0.218757	0.000519	0.222000	-2.035264	0.325981	
LiH	-0.787812	0.000083	0.091466	0.000086	0.092430	-0.605086	0.053909	
N2	-19.928185	0.000613	0.350251	0.000617	0.364600	-9.004438	0.387145	
N2H4	-22.255178	0.000375	0.677120	0.000388	0.699600	-14.106114	0.243589	1
NH	-10.417399	0.000228	0.128401	0.000232	0.133500	-3.199541	0.145362	

2.5.4 $\mu = 1/4$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.990898				12
C	-5.418170				7
Cl	-14.937611				11
F	-24.188208				8
H	-0.498899				1
Li	-0.198788				1
N	-9.786270				9
Na	-0.176097				1
O	-15.894795				6
P	-6.461580				41
S	-10.106026				6
Si	-3.759767				35
BeH	-1.558909	0.069111	0.079400	-6.456475	7
C2H2	-12.471698	0.637560	0.642400	-3.037220	198
C2H4	-13.726706	0.894768	0.899000	-2.655519	385
C2H6	-14.962823	1.133087	1.136900	-2.392704	2916
CH	-6.046905	0.129835	0.133900	-2.550684	7
$CH2_{1A1}$	-6.693768	0.277799	0.288900	-6.966033	8
$CH2_{3B1}$	-6.720192	0.304223	0.304100	0.077471	6
CH3	-7.402377	0.487509	0.490800	-2.065178	26
CH3Cl	-22.479630	0.627151	0.631000	-2.415124	1601
CH4	-8.077764	0.663997	0.670300	-3.955332	95
CN	-15.489681	0.285241	0.288800	-2.233465	171
CO	-21.724108	0.411144	0.413700	-1.604169	51
CO2	-37.837557	0.629798	0.621400	5.269703	184
CS	-15.789705	0.265510	0.274000	-5.327873	414
Cl2	-29.964137	0.088916	0.094000	-3.190568	394
ClF	-39.223298	0.097479	0.100100	-1.644539	20
ClO	-30.934485	0.102079	0.104700	-1.644598	101
F2	-48.443178	0.066763	0.062200	2.863228	8
H2CO	-22.908464	0.597700	0.596700	0.627571	193
H2O	-17.249751	0.357158	0.371900	-9.250928	8
H2O2	-33.205714	0.418325	0.429400	-6.949513	23
H2S	-11.384757	0.280933	0.292000	-6.944801	150
H3COH	-24.120733	0.812171	0.818700	-4.097129	1684
H3CSH	-18.266078	0.746285	0.757000	-6.723789	3354
HCN	-16.198560	0.495220	0.496900	-1.054027	200
HCO	-22.261161	0.449297	0.444700	2.884545	311
HCl	-15.601020	0.164510	0.171000	-4.072465	42
HF	-24.900836	0.213729	0.226100	-7.763223	10
HOCl	-31.588728	0.257423	0.264700	-4.566233	422
Li2	-0.427271	0.029694	0.038900	-5.776626	11
LiF	-24.598963	0.211967	0.222000	-6.295769	9
LiH	-0.784367	0.086680	0.092430	-3.608453	5
N2	-19.931576	0.359035	0.364600	-3.491877	48
N2H4	-22.254132	0.685994	0.699600	-8.537908	3322
NH	-10.417015	0.131845	0.133500	-1.038490	7

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		N
Be	-1.000950	0.000077	0.000000	0.000109				
C	-5.418125	0.000127	0.000000	0.000180				
Cl	-14.941712	0.000114	0.000000	0.000162				
F	-24.188728	0.000285	0.000000	0.000403				
H	-0.499992	0.000020	0.000000	0.000029				
Li	-0.196329	0.000015	0.000000	0.000021				
N	-9.788667	0.000111	0.000000	0.000157				
Na	-0.182037	0.000024	0.000000	0.000033				
O	-15.892785	0.000180	0.000000	0.000254				
P	-6.464300	0.000138	0.000000	0.000195				
S	-10.109068	0.000153	0.000000	0.000217				
Si	-3.759874	0.000098	0.000000	0.000139				
BeH	-1.577971	0.000128	0.077029	0.000151	0.079400	-1.487643	0.094552	
C2H2	-12.486730	0.000669	0.650496	0.000716	0.642400	5.080370	0.449548	1
C2H4	-13.741231	0.000683	0.905014	0.000733	0.899000	3.773550	0.460116	3
C2H6	-14.980526	0.000464	1.144325	0.000543	1.136900	4.659101	0.340885	29
CH	-6.049806	0.000150	0.131689	0.000197	0.133900	-1.387389	0.123828	
$CH2_{1A1}$	-6.705096	0.000214	0.286988	0.000252	0.288900	-1.200013	0.158314	
$CH2_{3B1}$	-6.725226	0.000143	0.307118	0.000196	0.304100	1.893573	0.122759	
CH3	-7.412609	0.000358	0.494508	0.000385	0.490800	2.326982	0.241282	
CH3Cl	-22.492399	0.000748	0.632586	0.000770	0.631000	0.995103	0.483283	16
CH4	-8.093244	0.000174	0.675152	0.000231	0.670300	3.044423	0.144710	
CN	-15.490160	0.000308	0.283368	0.000351	0.288800	-3.408539	0.220358	1
CO	-21.723377	0.000665	0.412467	0.000700	0.413700	-0.773921	0.439229	
CO2	-37.822849	0.000494	0.619154	0.000624	0.621400	-1.409325	0.391315	1
CS	-15.796844	0.000377	0.269651	0.000426	0.274000	-2.728813	0.267315	4
Cl2	-29.973351	0.000494	0.089927	0.000545	0.094000	-2.555890	0.341684	3
ClF	-39.219049	0.000920	0.088609	0.000970	0.100100	-7.210469	0.608396	
ClO	-30.924581	0.000543	0.090083	0.000583	0.104700	-9.172141	0.366117	1
F2	-48.421969	0.000420	0.044513	0.000708	0.062200	-11.098678	0.444069	
H2CO	-22.906726	0.000603	0.595833	0.000643	0.596700	-0.544331	0.403588	1
H2O	-17.253825	0.000305	0.361056	0.000356	0.371900	-6.804531	0.223570	
H2O2	-33.192631	0.000246	0.407077	0.000437	0.429400	-14.008183	0.274326	
H2S	-11.397763	0.000419	0.288711	0.000448	0.292000	-2.063710	0.281350	1
H3COH	-24.124458	0.000636	0.813580	0.000678	0.818700	-3.212607	0.425360	16
H3CSH	-18.283433	0.000546	0.756272	0.000587	0.757000	-0.456731	0.368206	33
HCN	-16.204158	0.000579	0.497375	0.000603	0.496900	0.297906	0.378384	2
HCO	-22.253647	0.000678	0.442745	0.000713	0.444700	-1.226619	0.447521	3
HCl	-15.611220	0.000442	0.169515	0.000457	0.171000	-0.931623	0.287064	
HF	-24.906153	0.000593	0.217433	0.000658	0.226100	-5.438329	0.412875	
HOCl	-31.587513	0.000397	0.253023	0.000451	0.264700	-7.327206	0.282720	4
Li2	-0.430261	0.000053	0.037603	0.000061	0.038900	-0.814136	0.038053	
LiF	-24.604507	0.000693	0.219450	0.000749	0.222000	-1.599960	0.470022	
LiH	-0.787972	0.000110	0.091651	0.000113	0.092430	-0.488719	0.070934	
N2	-19.931961	0.000410	0.354628	0.000467	0.364600	-6.257629	0.292981	
N2H4	-22.255192	0.000763	0.677891	0.000799	0.699600	-13.622919	0.501092	33
NH	-10.417875	0.000259	0.129216	0.000283	0.133500	-2.688057	0.177463	

2.5.5 $\mu = 1/2$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.992733				11
C	-5.424193				64
Cl	-14.936917				461
F	-24.211164				47
H	-0.502302				1
Li	-0.196387				1
N	-9.800001				55
Na	-0.174540				1
O	-15.911458				107
P	-6.459292				159
S	-10.103616				243
Si	-3.755570				129
BeH	-1.559665	0.064630	0.079400	-9.268590	123
C2H2	-12.471534	0.618546	0.642400	-14.968783	9728
C2H4	-13.729919	0.872327	0.899000	-16.737595	23964
C2H6	-14.972133	1.109937	1.136900	-16.919464	91784
CH	-6.051231	0.124737	0.133900	-5.750116	563
$CH2_{1A1}$	-6.698845	0.270049	0.288900	-11.829303	835
$CH2_{3B1}$	-6.727757	0.298961	0.304100	-3.224773	1246
CH3	-7.409416	0.478319	0.490800	-7.832194	1237
CH3Cl	-22.477835	0.609820	0.631000	-13.290489	49757
CH4	-8.084849	0.651450	0.670300	-11.828671	6627
CN	-15.486349	0.262155	0.288800	-16.719820	11031
CO	-21.730324	0.394674	0.413700	-11.939218	5235
CO2	-37.845033	0.597923	0.621400	-14.731778	36066
CS	-15.779785	0.251977	0.274000	-13.819555	24821
Cl2	-29.950545	0.076711	0.094000	-10.848822	12189
ClF	-39.229805	0.081725	0.100100	-11.530775	13567
ClO	-30.931179	0.082804	0.104700	-13.740165	12137
F2	-48.464871	0.042543	0.062200	-12.334916	1743
H2CO	-22.915457	0.575202	0.596700	-13.490053	11335
H2O	-17.262607	0.346545	0.371900	-15.910229	942
H2O2	-33.218344	0.390824	0.429400	-24.206976	30977
H2S	-11.381054	0.272835	0.292000	-12.026395	2744
H3COH	-24.134504	0.789646	0.818700	-18.231622	55296
H3CSH	-18.264445	0.727429	0.757000	-18.556005	212599
HCN	-16.198797	0.472302	0.496900	-15.435639	6486
HCO	-22.265861	0.427908	0.444700	-10.537012	26176
HCl	-15.598913	0.159695	0.171000	-7.094202	1519
HF	-24.921651	0.208185	0.226100	-11.241954	278
HOCl	-31.588809	0.238132	0.264700	-16.671508	25000
Li2	-0.428159	0.035385	0.038900	-2.205628	11
LiF	-24.616249	0.208698	0.222000	-8.347308	402
LiH	-0.783586	0.084897	0.092430	-4.726728	22
N2	-19.934126	0.334123	0.364600	-19.124792	3285
N2H4	-22.263550	0.654340	0.699600	-28.400957	96249
NH	-10.426427	0.124124	0.133500	-5.883439	571

2. DMC without Jastrow

	Total E Hartree		Delta E Hartree		Ref	Error kcal/mol	
Be	-1.005406	0.000017					
C	-5.422342	0.000063					
Cl	-14.949570	0.000204					
F	-24.189415	0.000167					
H	-0.499999	0.000005					
Li	-0.196328	0.000003					
N	-9.789680	0.000095					
Na	-0.182036	0.000014					
O	-15.893123	0.000111					
P	-6.467707	0.000099					
S	-10.115998	0.000111					
Si	-3.762843	0.000063					
C2H2	-12.489387	0.000584	0.644707	0.000598	0.642400	1.447461	0.375096
C2H4	-13.744276	0.000668	0.899598	0.000680	0.899000	0.375397	0.426707
C2H6	-14.983379	0.000770	1.138704	0.000781	1.136900	1.132012	0.490174
CH	-6.056035	0.000123	0.133695	0.000138	0.133900	-0.128821	0.086597
$CH2_{1A1}$	-6.711544	0.000153	0.289206	0.000166	0.288900	0.191740	0.103885
$CH2_{3B1}$	-6.727420	0.000148	0.305081	0.000161	0.304100	0.615573	0.101272
CH3	-7.413712	0.000178	0.491374	0.000189	0.490800	0.360485	0.118741
CH3Cl	-22.500012	0.000804	0.628105	0.000832	0.631000	-1.816343	0.521865
CH4	-8.094266	0.000377	0.671930	0.000383	0.670300	1.022969	0.240071
CN	-15.498861	0.000499	0.286838	0.000512	0.288800	-1.230928	0.321064
CO	-21.728832	0.000552	0.413368	0.000567	0.413700	-0.208251	0.355755
CO2	-37.823698	0.002088	0.615111	0.002100	0.621400	-3.946408	1.318062
CS	-15.809147	0.000535	0.270807	0.000550	0.274000	-2.003750	0.345077
Cl2	-29.987308	0.000616	0.088169	0.000739	0.094000	-3.659111	0.463821
ClF	-39.228251	0.000660	0.089267	0.000710	0.100100	-6.797869	0.445649
ClO	-30.935265	0.000858	0.092573	0.000889	0.104700	-7.609892	0.557853
F2	-48.428399	0.000642	0.049569	0.000723	0.062200	-7.926000	0.453759
H2CO	-22.911646	0.000726	0.596184	0.000738	0.596700	-0.323590	0.462837
H2O	-17.253919	0.000265	0.360799	0.000287	0.371900	-6.965878	0.180187
H2O2	-33.196548	0.000794	0.410305	0.000824	0.429400	-11.982031	0.517188
H2S	-11.403524	0.000238	0.287529	0.000263	0.292000	-2.805611	0.165046
H3COH	-24.125546	0.001003	0.810087	0.001011	0.818700	-5.404473	0.634540
H3CSH	-18.285601	0.002003	0.747267	0.002008	0.757000	-6.107676	1.259772
HCN	-16.208970	0.000638	0.496949	0.000648	0.496900	0.031033	0.406775
HCO	-22.257070	0.000696	0.441607	0.000708	0.444700	-1.940837	0.444111
HCl	-15.619019	0.000217	0.169451	0.000298	0.171000	-0.971823	0.186909
HF	-24.905752	0.000192	0.216339	0.000254	0.226100	-6.125233	0.159473
HOCl	-31.593260	0.002090	0.250570	0.002103	0.264700	-8.866896	1.319641
Li2	-0.431228	0.000009	0.038572	0.000011	0.038900	-0.206025	0.006888
LiF	-24.604326	0.000217	0.218583	0.000273	0.222000	-2.143995	0.171552
LiH	-0.787889	0.000024	0.091562	0.000024	0.092430	-0.544720	0.015313
N2	-19.936415	0.000503	0.357054	0.000538	0.364600	-4.735054	0.337403
N2H4	-22.257362	0.001121	0.678007	0.001137	0.699600	-13.549683	0.713532
NH	-10.418918	0.000163	0.129239	0.000189	0.133500	-2.673761	0.118450
NH2	-11.074786	0.000206	0.285108	0.000227	0.290400	-3.320737	0.142472

3. DMC

	Total E Hartree		Delta E Hartree		Ref	Error kcal/mol		N
Be	-1.005733	0.000012	0.000000	0.000018				
C	-5.422446	0.000070	0.000000	0.000100				
Cl	-14.949689	0.000087	0.000000	0.000122				
F	-24.188815	0.000114	0.000000	0.000161				
H	-0.499996	0.000007	0.000000	0.000010				
Li	-0.196329	0.000004	0.000000	0.000006				
N	-9.789676	0.000079	0.000000	0.000112				
Na	-0.182136	0.000008	0.000000	0.000011				
O	-15.893286	0.000064	0.000000	0.000091				
P	-6.467896	0.000077	0.000000	0.000109				
S	-10.115941	0.000074	0.000000	0.000104				
Si	-3.762860	0.000047	0.000000	0.000066				
BeH	-1.580444	0.000075	0.074715	0.000076	0.079400	-2.939685	0.047668	
C2H2	-12.491168	0.000383	0.646285	0.000408	0.642400	2.437853	0.256215	9
C2H4	-13.744599	0.000444	0.899725	0.000466	0.899000	0.455073	0.292715	23
C2H6	-14.983176	0.000623	1.138311	0.000640	1.136900	0.885531	0.401733	91
CH	-6.056197	0.000083	0.133756	0.000109	0.133900	-0.090328	0.068429	
$CH2_{1A1}$	-6.711440	0.000139	0.289004	0.000157	0.288900	0.064962	0.098268	
$CH2_{3B1}$	-6.727391	0.000143	0.304954	0.000160	0.304100	0.535803	0.100646	1
CH3	-7.413712	0.000127	0.491280	0.000147	0.490800	0.301192	0.092205	1
CH3Cl	-22.499891	0.000809	0.627770	0.000817	0.631000	-2.026712	0.512703	49
CH4	-8.093698	0.000266	0.671270	0.000276	0.670300	0.608405	0.173340	6
CN	-15.497971	0.000251	0.285850	0.000272	0.288800	-1.851206	0.170797	11
CO	-21.728259	0.000361	0.412527	0.000373	0.413700	-0.735981	0.234286	5
CO2	-37.827070	0.001289	0.618053	0.001297	0.621400	-2.100522	0.813791	36
CS	-15.807213	0.000434	0.268826	0.000446	0.274000	-3.246664	0.279694	24
Cl2	-29.987339	0.000995	0.087961	0.001010	0.094000	-3.789372	0.633674	12
ClF	-39.225577	0.000775	0.087074	0.000788	0.100100	-8.174187	0.494734	13
ClO	-30.934845	0.000499	0.091871	0.000511	0.104700	-8.050392	0.320560	12
F2	-48.424857	0.000827	0.047228	0.000857	0.062200	-9.394885	0.538069	1
H2CO	-22.912166	0.000600	0.596443	0.000608	0.596700	-0.161127	0.381237	11
H2O	-17.254291	0.000159	0.361014	0.000172	0.371900	-6.831237	0.107807	
H2O2	-33.194557	0.000902	0.407994	0.000911	0.429400	-13.432729	0.571901	30
H2S	-11.403508	0.000134	0.287577	0.000153	0.292000	-2.775745	0.096133	2
H3COH	-24.128469	0.000930	0.812755	0.000936	0.818700	-3.730536	0.587170	55
H3CSH	-18.289905	0.000597	0.751536	0.000607	0.757000	-3.428421	0.380612	212
HCN	-16.209503	0.000366	0.497386	0.000382	0.496900	0.305097	0.239420	6
HCO	-22.256546	0.000832	0.440819	0.000838	0.444700	-2.435571	0.525542	26
HCl	-15.618568	0.000238	0.168884	0.000254	0.171000	-1.328058	0.159119	1
HF	-24.905370	0.000150	0.216560	0.000189	0.226100	-5.986662	0.118575	
HOCl	-31.594348	0.000910	0.251377	0.000916	0.264700	-8.360050	0.574866	25
Li2	-0.431297	0.000010	0.038639	0.000013	0.038900	-0.163614	0.008245	
LiF	-24.603053	0.000218	0.217910	0.000246	0.222000	-2.566504	0.154164	
LiH	-0.788039	0.000016	0.091715	0.000018	0.092430	-0.448955	0.011471	
N2	-19.937268	0.000408	0.357917	0.000438	0.364600	-4.193666	0.274874	3
N2H4	-22.257960	0.000674	0.678627	0.000693	0.699600	-13.161038	0.434984	96
NH	-10.418942	0.000074	0.129271	0.000109	0.133500	-2.654017	0.068307	

2.5.6 $\mu = 1$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.997611				10
C	-5.420006				154
Cl	-14.923700				899
F	-24.213585				294
H	-0.500915				1
Li	-0.195702				1
N	-9.797528				118
Na	-0.174255				1
O	-15.905353				291
P	-6.454169				922
S	-10.093127				1126
Si	-3.752249				282
BeH	-1.556367	0.057841	0.079400	-13.528518	226
C2H2	-12.457919	0.616077	0.642400	-16.518135	421452
C2H4	-13.713486	0.869814	0.899000	-18.314755	3346530
C2H6	-14.952030	1.106528	1.136900	-19.058990	10660003
CH	-6.045004	0.124083	0.133900	-6.160218	1872
$CH2_{1A1}$	-6.693312	0.271476	0.288900	-10.933550	5231
$CH2_{3B1}$	-6.719689	0.297853	0.304100	-3.920345	4908
CH3	-7.400261	0.477510	0.490800	-8.339553	26089
CH3Cl	-22.453467	0.607016	0.631000	-15.050240	15279804
CH4	-8.076058	0.652392	0.670300	-11.237459	240746
CN	-15.473830	0.256296	0.288800	-20.396634	307534
CO	-21.713154	0.387795	0.413700	-16.255639	220058
CO2	-37.813665	0.582952	0.621400	-24.126272	10685733
CS	-15.764849	0.251716	0.274000	-13.983341	820828
Cl2	-29.919364	0.071964	0.094000	-13.828005	3156929
ClF	-39.205454	0.068169	0.100100	-20.037087	651358
ClO	-30.900816	0.071763	0.104700	-20.668394	1296735
F2	-48.446924	0.019754	0.062200	-26.635101	11952
H2CO	-22.894495	0.567305	0.596700	-18.445616	1357368
H2O	-17.252592	0.345408	0.371900	-16.623808	6136
H2O2	-33.189337	0.376800	0.429400	-33.006901	3209365
H2S	-11.368755	0.273798	0.292000	-11.421902	25567
H3COH	-24.111642	0.782622	0.818700	-22.639454	16305839
H3CSH	-18.240701	0.723907	0.757000	-20.765895	14045275
HCN	-16.182131	0.463682	0.496900	-20.844565	389108
HCO	-22.244739	0.418464	0.444700	-16.463310	1449983
HCl	-15.586327	0.161712	0.171000	-5.828337	12311
HF	-24.920723	0.206223	0.226100	-12.472870	1645
HOCl	-31.558798	0.228829	0.264700	-22.509312	3157539
Li2	-0.428740	0.037335	0.038900	-0.981967	20
LiF	-24.610269	0.200982	0.222000	-13.189002	3309
LiH	-0.780131	0.083514	0.092430	-5.595016	40
N2	-19.913827	0.318770	0.364600	-28.758523	94334
N2H4	-22.236209	0.637492	0.699600	-38.973422	12661156

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.007952	0.000012	0.000000	0.000016				
C	-5.429616	0.000033	0.000000	0.000047				
Cl	-14.957911	0.000125	0.000000	0.000176				
F	-24.189708	0.000075	0.000000	0.000106				
H	-0.499984	0.000020	0.000000	0.000029				
Li	-0.196348	0.000010	0.000000	0.000014				
N	-9.794416	0.000037	0.000000	0.000052				
Na	-0.182103	0.000035	0.000000	0.000050				
O	-15.895865	0.000051	0.000000	0.000073				
P	-6.471376	0.000041	0.000000	0.000059				
S	-10.122606	0.000038	0.000000	0.000054				
Si	-3.764793	0.000031	0.000000	0.000044				
BeH	-1.579250	0.000937	0.071314	0.000938	0.079400	-5.073920	0.588319	
C2H2	-12.495100	0.000288	0.635900	0.000299	0.642400	-4.078810	0.187395	
C2H4	-13.747119	0.000376	0.887951	0.000390	0.899000	-6.933248	0.244737	3
C2H6	-14.983968	0.000387	1.124832	0.000412	1.136900	-7.572876	0.258278	10
CH	-6.062427	0.000050	0.132827	0.000063	0.133900	-0.673247	0.039828	
$CH2_{1A1}$	-6.716232	0.000080	0.286648	0.000095	0.288900	-1.413201	0.059843	
$CH2_{3B1}$	-6.730644	0.000050	0.301060	0.000073	0.304100	-1.907457	0.045621	
CH3	-7.416019	0.000097	0.486452	0.000119	0.490800	-2.728686	0.074912	
CH3Cl	-22.506947	0.000469	0.619468	0.000490	0.631000	-7.236181	0.307687	15
CH4	-8.094626	0.000167	0.665074	0.000189	0.670300	-3.279230	0.118604	
CN	-15.506720	0.000166	0.282687	0.000173	0.288800	-3.835671	0.108781	
CO	-21.735455	0.000243	0.409974	0.000251	0.413700	-2.338246	0.157395	
CO2	-37.832076	0.000396	0.610730	0.000411	0.621400	-6.695775	0.257696	10
CS	-15.817846	0.000198	0.265623	0.000204	0.274000	-5.256451	0.128007	
Cl2	-30.001476	0.000279	0.085654	0.000374	0.094000	-5.236972	0.234638	3
ClF	-39.236680	0.000338	0.089061	0.000368	0.100100	-6.927034	0.230722	
ClO	-30.944753	0.000369	0.090977	0.000392	0.104700	-8.611150	0.246245	1
F2	-48.432448	0.000286	0.053032	0.000323	0.062200	-5.753097	0.202704	
H2CO	-22.915252	0.000192	0.589803	0.000205	0.596700	-4.327743	0.128890	1
H2O	-17.256766	0.000110	0.360933	0.000128	0.371900	-6.881910	0.080388	
H2O2	-33.200709	0.000311	0.409011	0.000330	0.429400	-12.794101	0.206847	3
H2S	-11.408516	0.000100	0.285942	0.000114	0.292000	-3.801350	0.071679	
H3COH	-24.129361	0.000463	0.803944	0.000474	0.818700	-9.259382	0.297326	16
H3CSH	-18.292741	0.000585	0.740583	0.000593	0.757000	-10.301775	0.372099	14
HCN	-16.216052	0.000231	0.492035	0.000237	0.496900	-3.052581	0.148532	
HCO	-22.261888	0.000225	0.436423	0.000234	0.444700	-5.193910	0.146899	1
HCl	-15.626549	0.000119	0.168654	0.000174	0.171000	-1.472062	0.108954	
HF	-24.905824	0.000099	0.216132	0.000126	0.226100	-6.255026	0.078940	
HOCl	-31.604341	0.000308	0.250581	0.000337	0.264700	-8.859634	0.211492	3
Li2	-0.431398	0.000031	0.038703	0.000036	0.038900	-0.123788	0.022885	
LiF	-24.603937	0.000137	0.217881	0.000157	0.222000	-2.584419	0.098261	
LiH	-0.788135	0.000087	0.091803	0.000090	0.092430	-0.393157	0.056186	
N2	-19.946437	0.000151	0.357604	0.000168	0.364600	-4.390231	0.105473	
N2H4	-22.262196	0.000381	0.673428	0.000397	0.699600	-16.423183	0.248963	12
NH	-10.423223	0.000077	0.128822	0.000088	0.133500	-2.935192	0.054979	

2.5.7 $\mu = 2$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.999854				20
C	-5.413512				256
Cl	-14.901401				8768
F	-24.167662				1123
H	-0.499395				1
Li	-0.195618				1
N	-9.777229				266
Na	-0.174229				1
O	-15.870717				720
P	-6.447040				883
S	-10.077913				2158
Si	-3.749526				280
BeH	-1.554506	0.055256	0.079400	-15.150357	233
C2H2	-12.433274	0.607460	0.642400	-21.924928	3536175
C2H4	-13.683977	0.859374	0.899000	-24.865914	13804446
C2H6	-14.914667	1.091274	1.136900	-28.630770	16695116
CH	-6.037897	0.124990	0.133900	-5.590831	4503
$CH2_{1A1}$	-6.684705	0.272403	0.288900	-10.351722	17886
$CH2_{3B1}$	-6.705455	0.293153	0.304100	-6.869315	26137
CH3	-7.383862	0.472165	0.490800	-11.693713	112935
CH3Cl	-22.409537	0.596440	0.631000	-21.687030	14187344
CH4	-8.058090	0.646999	0.670300	-14.621734	933450
CN	-15.449131	0.258390	0.288800	-19.082857	2523139
CO	-21.673981	0.389753	0.413700	-15.027166	1727262
CO2	-37.729909	0.574964	0.621400	-29.139318	11725352
CS	-15.741053	0.249628	0.274000	-15.293519	2658739
Cl2	-29.869270	0.066468	0.094000	-17.276448	12609257
ClF	-39.135766	0.066703	0.100100	-20.957172	8476468
ClO	-30.840649	0.068532	0.104700	-22.696037	10858948
F2	-48.359393	0.024069	0.062200	-23.927351	829438
H2CO	-22.846626	0.563608	0.596700	-20.765489	11090595
H2O	-17.214580	0.345073	0.371900	-16.834113	56247
H2O2	-33.116702	0.376479	0.429400	-33.208509	19069926
H2S	-11.348502	0.271799	0.292000	-12.676342	172622
H3COH	-24.054291	0.772483	0.818700	-29.001580	16136860
H3CSH	-18.200479	0.711474	0.757000	-28.567865	15981581
HCN	-16.152086	0.461950	0.496900	-21.931353	2869501
HCO	-22.198603	0.414979	0.444700	-18.650186	11562913
HCl	-15.561027	0.160232	0.171000	-6.757310	54420
HF	-24.873708	0.206651	0.226100	-12.204142	6415
HOCl	-31.496904	0.225391	0.264700	-24.666646	11555771
Li2	-0.428808	0.037571	0.038900	-0.833690	20
LiF	-24.561304	0.198023	0.222000	-15.045700	13192
LiH	-0.779366	0.084353	0.092430	-5.068416	43
N2	-19.879071	0.324613	0.364600	-25.092550	823923
N2H4	-22.180728	0.628690	0.699600	-44.496999	13428368

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.006595	0.000022						
C	-5.431906	0.000093						
Cl	-14.961958	0.000401						
F	-24.194111	0.000300						
H	-0.500001	0.000005						
Li	-0.196327	0.000003						
N	-9.798247	0.000123						
Na	-0.182031	0.000014						
O	-15.901191	0.000224						
P	-6.472694	0.000166						
S	-10.124398	0.000232						
Si	-3.765019	0.000078						
BeH	-1.578901	0.000071	0.072306	0.000075	0.079400	-4.451676	0.046990	
C2H2	-12.497788	0.000824	0.633975	0.000845	0.642400	-5.286650	0.530369	3
C2H4	-13.749666	0.001750	0.885851	0.001760	0.899000	-8.250839	1.104670	13
C2H6	-14.986264	0.001844	1.122449	0.001854	1.136900	-9.068419	1.163298	16
CH	-6.064139	0.000220	0.132232	0.000239	0.133900	-1.046559	0.149734	
$CH2_{1A1}$	-6.716863	0.000386	0.284956	0.000397	0.288900	-2.475141	0.249249	
$CH2_{3B1}$	-6.731490	0.000375	0.299583	0.000387	0.304100	-2.834312	0.242556	
CH3	-7.415891	0.000622	0.483984	0.000629	0.490800	-4.277356	0.394564	
CH3Cl	-22.511612	0.002044	0.617747	0.002085	0.631000	-8.316552	1.308100	14
CH4	-8.095004	0.000385	0.663096	0.000396	0.670300	-4.520816	0.248672	
CN	-15.513401	0.000697	0.283249	0.000714	0.288800	-3.483473	0.448137	2
CO	-21.741989	0.000808	0.408892	0.000844	0.413700	-3.017062	0.529316	1
CO2	-37.838563	0.002474	0.604275	0.002516	0.621400	-10.745815	1.578520	11
CS	-15.821184	0.000835	0.264880	0.000872	0.274000	-5.722774	0.547105	2
Cl2	-30.014456	0.001995	0.090541	0.002150	0.094000	-2.170680	1.349045	12
ClF	-39.243560	0.001936	0.087491	0.001999	0.100100	-7.912075	1.254574	8
ClO	-30.954676	0.001525	0.091528	0.001593	0.104700	-8.265845	0.999491	10
F2	-48.441060	0.000725	0.052839	0.000941	0.062200	-5.874238	0.590791	
H2CO	-22.916965	0.001482	0.583867	0.001502	0.596700	-8.052762	0.942212	11
H2O	-17.259101	0.000741	0.357910	0.000775	0.371900	-8.779163	0.486042	
H2O2	-33.204067	0.002796	0.401685	0.002831	0.429400	-17.391708	1.776731	19
H2S	-11.410534	0.000195	0.286135	0.000303	0.292000	-3.680234	0.190292	
H3COH	-24.132624	0.002133	0.799525	0.002147	0.818700	-12.032629	1.347382	16
H3CSH	-18.298936	0.002118	0.742630	0.002133	0.757000	-9.017169	1.338446	15
HCN	-16.220587	0.000843	0.490434	0.000857	0.496900	-4.057275	0.537619	2
HCO	-22.267292	0.001637	0.434195	0.001655	0.444700	-6.591982	1.038261	11
HCl	-15.629973	0.000818	0.168015	0.000911	0.171000	-1.873090	0.571667	
HF	-24.910279	0.000519	0.216168	0.000600	0.226100	-6.232372	0.376339	
HOCl	-31.613092	0.002201	0.249943	0.002248	0.264700	-9.260126	1.410753	11
Li2	-0.431190	0.000014	0.038535	0.000015	0.038900	-0.229050	0.009272	
LiF	-24.608427	0.000670	0.217989	0.000735	0.222000	-2.516888	0.460954	
LiH	-0.788722	0.000024	0.092394	0.000025	0.092430	-0.022762	0.015673	
N2	-19.952444	0.000503	0.355951	0.000560	0.364600	-5.427264	0.351126	
N2H4	-22.269791	0.002112	0.673296	0.002126	0.699600	-16.506001	1.334261	13
NH	-10.426399	0.000367	0.128152	0.000387	0.133500	-3.355986	0.242715	

2.5.8 $\mu = 5$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-1.000376				20
C	-5.410380				263
Cl	-14.881046				6494
F	-24.111984				2062
H	-0.499061				1
Li	-0.195612				1
N	-9.763552				541
Na	-0.174227				1
O	-15.839365				2128
P	-6.443065				887
S	-10.067504				4574
Si	-3.748107				278
BeH	-1.553839	0.054402	0.079400	-15.686777	233
C2H2	-12.412686	0.593804	0.642400	-30.494351	6437284
C2H4	-13.660002	0.842998	0.899000	-35.141559	10042908
C2H6	-14.886209	1.071084	1.136900	-41.300048	15548822
CH	-6.032511	0.123070	0.133900	-6.795753	4563
$CH2_{1A1}$	-6.677066	0.268564	0.288900	-12.760815	33173
$CH2_{3B1}$	-6.696022	0.287520	0.304100	-10.404092	32666
CH3	-7.371993	0.464431	0.490800	-16.547001	164563
CH3Cl	-22.373709	0.585101	0.631000	-28.802093	14867432
CH4	-8.044466	0.637844	0.670300	-20.366729	1872343
CN	-15.427312	0.253380	0.288800	-22.226397	4111066
CO	-21.633999	0.384253	0.413700	-18.478174	3069921
CO2	-37.647268	0.558157	0.621400	-39.685566	10668509
CS	-15.721648	0.243764	0.274000	-18.973595	4545205
Cl2	-29.825298	0.063206	0.094000	-19.323669	10038408
ClF	-39.059718	0.066688	0.100100	-20.966267	12928114
ClO	-30.786196	0.065784	0.104700	-24.420007	12144026
F2	-48.257292	0.033324	0.062200	-18.120087	5326459
H2CO	-22.801548	0.553681	0.596700	-26.994596	11136605
H2O	-17.177034	0.339547	0.371900	-20.301762	109105
H2O2	-33.047087	0.370234	0.429400	-37.127006	10985101
H2S	-11.332958	0.267332	0.292000	-15.479475	256788
H3COH	-24.003383	0.757394	0.818700	-38.469859	17678584
H3CSH	-18.170900	0.696772	0.757000	-37.793392	16397010
HCN	-16.125520	0.452528	0.496900	-27.844052	5180719
HCO	-22.155268	0.406462	0.444700	-23.994747	12216859
HCl	-15.538103	0.157996	0.171000	-8.160063	97332
HF	-24.815328	0.204283	0.226100	-13.690103	27889
HOCl	-31.440622	0.221149	0.264700	-27.328400	17238463
Li2	-0.428786	0.037563	0.038900	-0.839265	20
LiF	-24.503400	0.195804	0.222000	-16.438369	28554
LiH	-0.779351	0.084679	0.092430	-4.863917	42
N2	-19.846393	0.319289	0.364600	-28.432826	1768856
N2H4	-22.135439	0.612093	0.699600	-54.911647	14198240

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Na	-0.182031	0.000014						
Li	-0.196327	0.000003						
Be	-1.006664	0.000023						
C	-5.431907	0.000095						
F	-24.194681	0.000375						
H	-0.500001	0.000005						
O	-15.900981	0.000287						
N	-9.798393	0.000165						
P	-6.472602	0.000169						
Si	-3.765070	0.000086						
Cl	-14.961838	0.000389						
S	-10.124174	0.000246						
BeH	-1.578740	0.000073	0.072075	0.000077	0.079400	-4.596315	0.048049	
C2H2	-12.495567	0.000935	0.631751	0.000955	0.642400	-6.682460	0.599080	6
C2H4	-13.747247	0.001348	0.883430	0.001362	0.899000	-9.770419	0.854619	10
C2H6	-14.983154	0.001875	1.119336	0.001885	1.136900	-11.021494	1.182746	15
CH	-6.063608	0.000221	0.131700	0.000241	0.133900	-1.380442	0.151133	
$CH2_{1A1}$	-6.716850	0.000513	0.284942	0.000522	0.288900	-2.483772	0.327298	
$CH2_{3B1}$	-6.731493	0.000407	0.299585	0.000418	0.304100	-2.833394	0.262557	
CH3	-7.415403	0.000733	0.483494	0.000739	0.490800	-4.584446	0.463978	
CH3Cl	-22.512288	0.002038	0.618541	0.002077	0.631000	-7.818214	1.303594	14
CH4	-8.094119	0.000507	0.662210	0.000517	0.670300	-5.076674	0.324265	1
CN	-15.511895	0.000794	0.281595	0.000817	0.288800	-4.521172	0.512399	4
CO	-21.740734	0.000859	0.407845	0.000910	0.413700	-3.673902	0.571331	3
CO2	-37.835298	0.002356	0.601428	0.002427	0.621400	-12.532638	1.522941	10
CS	-15.822427	0.001073	0.266345	0.001105	0.274000	-4.803354	0.693625	4
Cl2	-30.012216	0.001912	0.088540	0.002064	0.094000	-3.426197	1.295187	10
ClF	-39.245174	0.002160	0.088654	0.002227	0.100100	-7.182356	1.397462	12
ClO	-30.954136	0.001757	0.091317	0.001822	0.104700	-8.398101	1.143378	12
F2	-48.445320	0.002051	0.055957	0.002184	0.062200	-3.917423	1.370273	5
H2CO	-22.916768	0.001622	0.583878	0.001650	0.596700	-8.045842	1.035418	11
H2O	-17.258077	0.000196	0.357095	0.000348	0.371900	-9.290509	0.218178	
H2O2	-33.210332	0.002973	0.408368	0.003028	0.429400	-13.197551	1.900072	10
H2S	-11.410339	0.000216	0.286164	0.000328	0.292000	-3.662245	0.205664	
H3COH	-24.130840	0.000815	0.797949	0.000869	0.818700	-13.021543	0.545607	17
H3CSH	-18.297173	0.002210	0.741090	0.002226	0.757000	-9.983954	1.396599	16
HCN	-16.219231	0.001067	0.488930	0.001084	0.496900	-5.001235	0.680359	5
HCO	-22.263419	0.001572	0.430530	0.001601	0.444700	-8.891761	1.004345	12
HCl	-15.630285	0.000882	0.168446	0.000964	0.171000	-1.602747	0.605229	
HF	-24.908712	0.000747	0.214030	0.000835	0.226100	-7.574232	0.524267	
HOCl	-31.616639	0.002357	0.253819	0.002406	0.264700	-6.827851	1.509663	17
Li2	-0.431197	0.000014	0.038543	0.000015	0.038900	-0.224216	0.009263	
LiF	-24.607924	0.000805	0.216915	0.000888	0.222000	-3.190759	0.557103	
LiH	-0.788570	0.000027	0.092242	0.000028	0.092430	-0.117848	0.017467	
N2	-19.949524	0.000705	0.352738	0.000778	0.364600	-7.443594	0.488192	1
N2H4	-22.264424	0.000801	0.667636	0.000867	0.699600	-20.057903	0.543954	14
NH	-10.425639	0.000387	0.127246	0.000421	0.133500	-3.924735	0.264033	

2.5.9 FCI

1. CIPSI

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
	e_{cal}	ae_{cal}	ae_{nr}	ae_{diff}	Ndet		
Be	-1.000525	0.000000	0.000000	0.000000			
C	-5.409599	0.000005	0.000000	0.000008			
Cl	-14.874672	0.000003	0.000000	0.000004			
F	-24.092714	0.000002	0.000000	0.000003			
H	-0.499045	0.000000		0.000000			
Li	-0.195611	0.000000		0.000000			
N	-9.760495	0.000004	0.000000	0.000006			
Na	-0.174227	0.000000		0.000000			
O	-15.830021	0.000005	0.000000	0.000007			
P	-6.442099	0.000004	0.000000	0.000006			
S	-10.064311	0.000002	0.000000	0.000002			
Si	-3.747833	0.000004	0.000000	0.000005			
BeH	-1.553657	0.000020	0.054087	0.000020	0.079400	-15.884299	0.012745
C2H2	-12.406315	0.000001	0.589027	0.000011	0.642400	-33.492129	0.006743
C2H4	-13.654309	0.000006	0.838930	0.000012	0.899000	-37.694551	0.007803
C2H6	-14.883546	0.000042	1.070077	0.000043	1.136900	-41.932051	0.027188
CH	-6.030934	0.000018	0.122290	0.000018	0.133900	-7.285247	0.011601
$CH2_{1A1}$	-6.674394	0.000001	0.266704	0.000005	0.288900	-13.927911	0.003396
$CH2_{3B1}$	-6.693528	0.000006	0.285839	0.000008	0.304100	-11.459136	0.005163
CH3	-7.368566	0.000005	0.461832	0.000007	0.490800	-18.177798	0.004427
CH3Cl	-22.365840	0.000001	0.584434	0.000006	0.631000	-29.220712	0.003816
CH4	-8.040305	0.000000	0.634525	0.000005	0.670300	-22.449252	0.003365
CN	-15.420598	0.000003	0.250504	0.000007	0.288800	-24.031255	0.004544
CO	-21.620628	0.000002	0.381008	0.000008	0.413700	-20.514513	0.004735
CO2	-37.628607	0.000059	0.558965	0.000060	0.621400	-39.178355	0.037402
CS	-15.715859	0.000007	0.241949	0.000009	0.274000	-20.112329	0.005672
Cl2	-29.813093	0.000027	0.063750	0.000028	0.094000	-18.982410	0.017322
ClF	-39.034069	0.000003	0.066683	0.000005	0.100100	-20.969596	0.003000
ClO	-30.770680	0.000045	0.065986	0.000045	0.104700	-24.293159	0.028395
F2	-48.220437	0.000013	0.035009	0.000014	0.062200	-17.062405	0.008592
H2CO	-22.787835	0.000007	0.550124	0.000010	0.596700	-29.226623	0.006371
H2O	-17.164687	0.000002	0.336575	0.000005	0.371900	-22.166891	0.003427
H2O2	-33.028440	0.000005	0.370306	0.000011	0.429400	-37.081794	0.007070
H2S	-11.328294	0.000005	0.265892	0.000005	0.292000	-16.382937	0.003348
H3COH	-23.991233	0.000031	0.755432	0.000032	0.818700	-39.701171	0.019791
H3CSH	-18.167969	0.000012	0.697878	0.000013	0.757000	-37.099583	0.008264
HCN	-16.117018	0.000010	0.447879	0.000012	0.496900	-30.761212	0.007333
HCO	-22.143045	0.000045	0.404380	0.000045	0.444700	-25.301260	0.028375
HCl	-15.530706	0.000002	0.156989	0.000004	0.171000	-8.791842	0.002203
HF	-24.794339	0.000004	0.202580	0.000004	0.226100	-14.759161	0.002800
HOCl	-31.423913	0.000024	0.220175	0.000024	0.264700	-27.940178	0.015246
Li2	-0.429044	0.000060	0.037821	0.000060	0.038900	-0.676813	0.037575
LiF	-24.483187	0.000002	0.194861	0.000003	0.222000	-17.029906	0.001685
LiH	-0.779445	0.000017	0.084788	0.000017	0.092430	-4.795199	0.010737
N2	-19.835407	0.000003	0.314416	0.000009	0.364600	-31.491175	0.005555

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.007625	0.000014	0.000000	0.000020				
C	-5.431715	0.000065	0.000000	0.000092				
Cl	-14.962307	0.000256	0.000000	0.000362				
F	-24.193487	0.000257	0.000000	0.000363				
H	-0.499996	0.000007	0.000000	0.000010				
Li	-0.196329	0.000004	0.000000	0.000006				
N	-9.798226	0.000105	0.000000	0.000149				
Na	-0.182136	0.000008	0.000000	0.000011				
O	-15.900621	0.000176	0.000000	0.000249				
P	-6.472697	0.000089	0.000000	0.000126				
S	-10.124922	0.000191	0.000000	0.000271				
Si	-3.765137	0.000063	0.000000	0.000089				
BeH	-1.579924	0.000058	0.072304	0.000060	0.079400	-4.452718	0.037652	
C2H2	-12.491177	0.001978	0.627755	0.001982	0.642400	-9.189949	1.243661	6
C2H4	-13.747858	0.002165	0.884445	0.002169	0.899000	-9.133250	1.360919	10
C2H6	-14.980890	0.002993	1.117486	0.002996	1.136900	-12.182781	1.880250	17
CH	-6.063309	0.000142	0.131598	0.000156	0.133900	-1.444348	0.098110	
$CH2_{1A1}$	-6.715937	0.000274	0.284230	0.000282	0.288900	-2.930337	0.176733	
$CH2_{3B1}$	-6.730926	0.000247	0.299220	0.000256	0.304100	-3.062465	0.160633	
CH3	-7.415930	0.000433	0.484228	0.000439	0.490800	-4.124162	0.275260	
CH3Cl	-22.511728	0.003261	0.617719	0.003272	0.631000	-8.333880	2.053169	15
CH4	-8.092352	0.001733	0.660654	0.001735	0.670300	-6.052881	1.088669	3
CN	-15.511536	0.001716	0.281595	0.001721	0.288800	-4.521091	1.079775	4
CO	-21.740502	0.002046	0.408166	0.002055	0.413700	-3.472682	1.289362	3
CO2	-37.838828	0.001777	0.605871	0.001812	0.621400	-9.744893	1.137305	14
CS	-15.809393	0.002280	0.252755	0.002289	0.274000	-13.331407	1.436248	4
Cl2	-30.006770	0.001417	0.082156	0.001507	0.094000	-7.432073	0.945753	12
ClF	-39.247103	0.001471	0.091309	0.001515	0.100100	-5.516449	0.950520	12
ClO	-30.948491	0.002849	0.085563	0.002866	0.104700	-12.008590	1.798595	10
F2	-48.437580	0.002788	0.050606	0.002835	0.062200	-7.275352	1.779096	8
H2CO	-22.914591	0.002667	0.582263	0.002674	0.596700	-9.059348	1.677865	10
H2O	-17.257153	0.000554	0.356541	0.000582	0.371900	-9.637832	0.365219	
H2O2	-33.210861	0.001813	0.409628	0.001847	0.429400	-12.406998	1.158935	10
H2S	-11.410576	0.000694	0.285663	0.000720	0.292000	-3.976713	0.451833	
H3COH	-24.133288	0.001467	0.800970	0.001480	0.818700	-11.126046	0.928505	16
H3CSH	-18.293307	0.003131	0.736687	0.003138	0.757000	-12.746473	1.969176	18
HCN	-16.216313	0.002143	0.486376	0.002146	0.496900	-6.603748	1.346757	8
HCO	-22.262328	0.002545	0.429996	0.002552	0.444700	-9.226696	1.601523	12
HCl	-15.630053	0.000503	0.167751	0.000564	0.171000	-2.039062	0.354034	
HF	-24.908111	0.000426	0.214628	0.000498	0.226100	-7.198764	0.312367	
HOCl	-31.608392	0.001374	0.245468	0.001409	0.264700	-12.068155	0.883968	10
Li2	-0.431300	0.000009	0.038642	0.000012	0.038900	-0.162060	0.007643	
LiF	-24.606552	0.000507	0.216736	0.000568	0.222000	-3.303261	0.356414	
LiH	-0.788098	0.000017	0.091774	0.000019	0.092430	-0.411737	0.011790	
N2	-19.949099	0.001829	0.352648	0.001841	0.364600	-7.499767	1.155305	2
N2H4	-22.254991	0.001486	0.658557	0.001501	0.699600	-25.754667	0.941605	13
NH	-10.425927	0.000232	0.127706	0.000255	0.133500	-3.635724	0.159726	

2.5.10 Optimal mu

1. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
Be	-1.007961	0.000022	0.000000	0.000031			
C	-5.432014	0.000206	0.000000	0.000291			
Cl	-14.962307	0.000512	0.000000	0.000724			
F	-24.194931	0.000739	0.000000	0.001045			
H	-0.500031	0.000036	0.000000	0.000051			
Li	-0.196348	0.000020	0.000000	0.000028			
N	-9.798642	0.000312	0.000000	0.000441			
Na	-0.182144	0.000028	0.000000	0.000039			
O	-15.901711	0.000538	0.000000	0.000761			
P	-6.472749	0.000369	0.000000	0.000522			
S	-10.124922	0.000382	0.000000	0.000540			
Si	-3.765137	0.000126	0.000000	0.000178			
BeH	-1.580516	0.000407	0.072524	0.000409	0.079400	-4.314947	0.256635
C2H2	-12.497801	0.001694	0.633712	0.001745	0.642400	-5.451619	1.094747
C2H4	-13.749665	0.003523	0.885514	0.003550	0.899000	-8.462788	2.227753
C2H6	-14.986262	0.003724	1.122049	0.003753	1.136900	-9.319339	2.355190
CH	-6.064142	0.000457	0.132097	0.000503	0.133900	-1.131338	0.315606
$CH2_{1A1}$	-6.716895	0.001010	0.284820	0.001033	0.288900	-2.560366	0.648276
$CH2_{3B1}$	-6.731543	0.000876	0.299468	0.000903	0.304100	-2.906815	0.566781
CH3	-7.416230	0.000531	0.484123	0.000580	0.490800	-4.189759	0.363707
CH3Cl	-22.512392	0.004245	0.617978	0.004282	0.631000	-8.171121	2.686994
CH4	-8.095023	0.000712	0.662886	0.000755	0.670300	-4.652422	0.473859
CN	-15.513658	0.001488	0.283003	0.001534	0.288800	-3.637926	0.962760
CO	-21.742290	0.001696	0.408566	0.001792	0.413700	-3.221762	1.124209
CO2	-37.838828	0.003554	0.603393	0.003719	0.621400	-11.299761	2.333710
CS	-15.822821	0.002003	0.265885	0.002050	0.274000	-5.091993	1.286195
Cl2	-30.015282	0.004435	0.090668	0.004552	0.094000	-2.090801	2.856122
ClF	-39.247103	0.002942	0.089865	0.003076	0.100100	-6.422439	1.930442
ClO	-30.955721	0.003402	0.091703	0.003482	0.104700	-8.155936	2.184944
F2	-48.445326	0.004050	0.055464	0.004311	0.062200	-4.226845	2.705490
H2CO	-22.917150	0.003311	0.583364	0.003361	0.596700	-8.368473	2.109226
H2O	-17.259143	0.001461	0.357370	0.001559	0.371900	-9.117846	0.978175
H2O2	-33.212019	0.004670	0.408535	0.004793	0.429400	-13.092808	3.007386
H2S	-11.410615	0.000390	0.285631	0.000551	0.292000	-3.996862	0.345646
H3COH	-24.133288	0.002934	0.799440	0.002993	0.818700	-12.086094	1.878439
H3CSH	-18.299331	0.004557	0.742272	0.004580	0.757000	-9.242030	2.873786
HCN	-16.220753	0.001826	0.490066	0.001864	0.496900	-4.288152	1.169733
HCO	-22.267303	0.003310	0.433548	0.003360	0.444700	-6.997992	2.108374
HCl	-15.630371	0.001893	0.168033	0.001961	0.171000	-1.861759	1.230832
HF	-24.910464	0.001192	0.215502	0.001403	0.226100	-6.650163	0.880384
HOCl	-31.616696	0.004825	0.252648	0.004882	0.264700	-7.563064	3.063237
Li2	-0.431467	0.000036	0.038771	0.000054	0.038900	-0.081074	0.033797
LiF	-24.608829	0.001551	0.217551	0.001718	0.222000	-2.792043	1.078202
LiH	-0.788766	0.000031	0.092387	0.000051	0.092430	-0.027234	0.032164
N2	-19.952486	0.001049	0.355202	0.001220	0.364600	-5.897402	0.765867
N2H4	-22.269902	0.004249	0.672494	0.004297	0.699600	-17.009600	2.696656

2.6 VTZ-BFD

2.6.1 CCSD(T)

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-1.008436			
C	-5.427472			
Cl	-14.945398			
F	-24.163293			
H	-0.499043			
Li	-0.196093			
N	-9.790590			
Na	-0.181799			
O	-15.882204			
P	-6.468767			
S	-10.115047			
Si	-3.762765			
BeH	-1.581711	0.074232	0.079400	-3.242985
C2H2	-12.478674	0.625645	0.642400	-10.513868
C2H4	-13.727519	0.876404	0.899000	-14.179031
C2H6	-14.960797	1.111596	1.136900	-15.878341
CH	-6.056141	0.129627	0.133900	-2.681602
$CH2_{1A1}$	-6.705994	0.280436	0.288900	-5.311028
$CH2_{3B1}$	-6.722273	0.296716	0.304100	-4.633521
CH3	-7.404435	0.479834	0.490800	-6.880995
CH3Cl	-22.480675	0.610676	0.631000	-12.753600
CH4	-8.080865	0.657222	0.670300	-8.206828
CN	-15.488160	0.270098	0.288800	-11.735518
CO	-21.710194	0.400519	0.413700	-8.271300
CO2	-37.788022	0.596143	0.621400	-15.849245
CS	-15.802251	0.259732	0.274000	-8.953503
Cl2	-29.974170	0.083373	0.094000	-6.668402
ClF	-39.196743	0.088052	0.100100	-7.560187
ClO	-30.917944	0.090342	0.104700	-9.010093
F2	-48.379472	0.052887	0.062200	-5.843976
H2CO	-22.885687	0.577926	0.596700	-11.781052
H2O	-17.231656	0.351366	0.371900	-12.885154
H2O2	-33.161842	0.399349	0.429400	-18.857479
H2S	-11.395638	0.282505	0.292000	-5.958152
H3COH	-24.096496	0.790649	0.818700	-17.602030
H3CSH	-18.271027	0.732336	0.757000	-15.476709
HCN	-16.195829	0.478724	0.496900	-11.405350
HCO	-22.235478	0.426760	0.444700	-11.257525
HCl	-15.609599	0.165158	0.171000	-3.665860
HF	-24.873550	0.211214	0.226100	-9.341166
HOCl	-31.571555	0.244910	0.264700	-12.418209
Li2	-0.431324	0.039137	0.038900	0.148744
LiF	-24.571797	0.212411	0.222000	-6.016966
LiH	-0.786075	0.090939	0.092430	-0.935801

2.6.2 DFT

1. PBE

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.995991			
C	-5.419118			
Cl	-14.944194			
F	-24.193196			
H	-0.497460			
Li	-0.200687			
N	-9.787241			
Na	-0.187487			
O	-15.899796			
P	-6.463623			
S	-10.113356			
Si	-3.765007			
BeH	-1.580650	0.087199	0.079400	4.894017
C2H2	-12.486965	0.653810	0.642400	7.159796
C2H4	-13.735055	0.906981	0.899000	5.007887
C2H6	-14.964553	1.141559	1.136900	2.923734
CH	-6.051717	0.135139	0.133900	0.777688
$CH2_{1A1}$	-6.697363	0.283326	0.288900	-3.497800
$CH2_{3B1}$	-6.728559	0.314522	0.304100	6.539772
CH3	-7.408198	0.496701	0.490800	3.702898
CH3Cl	-22.488662	0.632970	0.631000	1.236350
CH4	-8.079635	0.670679	0.670300	0.237715
CN	-15.509687	0.303328	0.288800	9.116634
CO	-21.732795	0.413881	0.413700	0.113545
CO2	-37.857917	0.639206	0.621400	11.173671
CS	-15.808394	0.275919	0.274000	1.204396
Cl2	-29.988660	0.100271	0.094000	3.935165
ClF	-39.243727	0.106336	0.100100	3.913345
ClO	-30.962770	0.118780	0.104700	8.835315
F2	-48.457231	0.070838	0.062200	5.420598
H2CO	-22.917097	0.603264	0.596700	4.118822
H2O	-17.252686	0.357971	0.371900	-8.740856
H2O2	-33.216050	0.421539	0.429400	-4.932762
H2S	-11.396219	0.287944	0.292000	-2.545448
H3COH	-24.124195	0.815443	0.818700	-2.043976
H3CSH	-18.279257	0.756944	0.757000	-0.034932
HCN	-16.211030	0.507212	0.496900	6.470739
HCO	-22.272333	0.455960	0.444700	7.065490
HCl	-15.608881	0.167227	0.171000	-2.367787
HF	-24.903909	0.213253	0.226100	-8.061664
HOCl	-31.605991	0.264541	0.264700	-0.100055
Li2	-0.428730	0.027355	0.038900	-7.244695
LiF	-24.607418	0.213534	0.222000	-5.312317
LiH	-0.783761	0.085614	0.092430	-4.277016
N2	-19.944031	0.369549	0.364600	3.105646
N2H4	-22.260667	0.696348	0.699600	-2.040800
NH	-10.424248	0.139547	0.133500	3.794796

2. BLYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.990724			
C	-5.412035			
Cl	-14.919266			
F	-24.195703			
H	-0.495143			
Li	-0.196415			
N	-9.773575			
Na	-0.183293			
O	-15.895611			
P	-6.436111			
S	-10.087796			
Si	-3.745916			
BeH	-1.576501	0.090634	0.079400	7.049468
C2H2	-12.442751	0.628395	0.642400	-8.788532
C2H4	-13.683411	0.878768	0.899000	-12.695652
C2H6	-14.904358	1.109429	1.136900	-17.238068
CH	-6.042774	0.135595	0.133900	1.063769
$CH2_{1A1}$	-6.685429	0.283108	0.288900	-3.634447
$CH2_{3B1}$	-6.705222	0.302901	0.304100	-0.752635
CH3	-7.384027	0.486563	0.490800	-2.659044
CH3Cl	-22.426873	0.610143	0.631000	-13.088176
CH4	-8.051779	0.659172	0.670300	-6.983033
CN	-15.473092	0.287482	0.288800	-0.826773
CO	-21.705111	0.397465	0.413700	-10.187534
CO2	-37.806732	0.603475	0.621400	-11.248075
CS	-15.760496	0.260665	0.274000	-8.367819
Cl2	-29.925185	0.086653	0.094000	-4.610273
ClF	-39.211343	0.096374	0.100100	-2.338174
ClO	-30.921408	0.106531	0.104700	1.148990
F2	-48.456313	0.064907	0.062200	1.698944
H2CO	-22.881225	0.583293	0.596700	-8.413018
H2O	-17.237978	0.352081	0.371900	-12.436373
H2O2	-33.189432	0.407925	0.429400	-13.475759
H2S	-11.363324	0.285243	0.292000	-4.240357
H3COH	-24.080384	0.792166	0.818700	-16.650319
H3CSH	-18.213982	0.733579	0.757000	-14.696914
HCN	-16.172336	0.491583	0.496900	-3.336267
HCO	-22.239825	0.437036	0.444700	-4.809541
HCl	-15.578024	0.163615	0.171000	-4.634269
HF	-24.900105	0.209259	0.226100	-10.568046
HOCl	-31.560892	0.250872	0.264700	-8.677149
Li2	-0.423039	0.030210	0.038900	-5.453102
LiF	-24.606894	0.214776	0.222000	-4.533028
LiH	-0.786019	0.094462	0.092430	1.274872
N2	-19.908692	0.361542	0.364600	-1.918770
N2H4	-22.209436	0.681714	0.699600	-11.223336
NH	-10.409081	0.140364	0.133500	4.306933

3. PBE0

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.997403			
C	-5.421836			
Cl	-14.950473			
F	-24.191931			
H	-0.499425			
Li	-0.201027			
N	-9.791806			
Na	-0.187580			
O	-15.900347			
P	-6.467784			
S	-10.118287			
Si	-3.766385			
BeH	-1.583607	0.086779	0.079400	4.630417
C2H2	-12.483540	0.641017	0.642400	-0.867601
C2H4	-13.738962	0.897589	0.899000	-0.885439
C2H6	-14.976908	1.136684	1.136900	-0.135562
CH	-6.053762	0.132501	0.133900	-0.878119
$CH2_{1A1}$	-6.700648	0.279961	0.288900	-5.609285
$CH2_{3B1}$	-6.733658	0.312971	0.304100	5.566845
CH3	-7.414741	0.494629	0.490800	2.402552
CH3Cl	-22.497175	0.626590	0.631000	-2.767530
CH4	-8.087640	0.668102	0.670300	-1.378975
CN	-15.491495	0.277853	0.288800	-6.869428
CO	-21.719381	0.397198	0.413700	-10.355225
CO2	-37.829845	0.607314	0.621400	-8.839069
CS	-15.800526	0.260403	0.274000	-8.532254
Cl2	-29.992501	0.091554	0.094000	-1.534621
ClF	-39.232663	0.090259	0.100100	-6.175081
ClO	-30.950426	0.099605	0.104700	-3.196895
F2	-48.427906	0.044044	0.062200	-11.392800
H2CO	-22.906759	0.585725	0.596700	-6.886885
H2O	-17.248357	0.349159	0.371900	-14.270335
H2O2	-33.195453	0.395908	0.429400	-21.016443
H2S	-11.401668	0.284530	0.292000	-4.687354
H3COH	-24.122893	0.803008	0.818700	-9.846612
H3CSH	-18.287977	0.750152	0.757000	-4.297097
HCN	-16.200224	0.487156	0.496900	-6.114165
HCO	-22.258027	0.436419	0.444700	-5.196545
HCl	-15.614960	0.165061	0.171000	-3.726559
HF	-24.898354	0.206998	0.226100	-11.986513
HOCl	-31.597823	0.247577	0.264700	-10.744900
Li2	-0.429693	0.027640	0.038900	-7.065499
LiF	-24.596813	0.203856	0.222000	-11.385494
LiH	-0.784788	0.084336	0.092430	-5.079099
N2	-19.928903	0.345292	0.364600	-12.116270
N2H4	-22.257466	0.676153	0.699600	-14.713280
NH	-10.425865	0.134634	0.133500	0.711350

4. B3LYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-1.001064			
C	-5.432579			
Cl	-14.960253			
F	-24.226363			
H	-0.500247			
Li	-0.200497			
N	-9.801065			
Na	-0.187080			
O	-15.923078			
P	-6.464760			
S	-10.122081			
Si	-3.766551			
BeH	-1.592187	0.090876	0.079400	7.201446
C2H2	-12.494274	0.628623	0.642400	-8.645039
C2H4	-13.751531	0.885387	0.899000	-8.542116
C2H6	-14.989941	1.123304	1.136900	-8.531671
CH	-6.068218	0.135393	0.133900	0.936957
$CH2_{1A1}$	-6.718234	0.285162	0.288900	-2.345487
$CH2_{3B1}$	-6.738986	0.305914	0.304100	1.138201
CH3	-7.424792	0.491474	0.490800	0.422772
CH3Cl	-22.509544	0.615972	0.631000	-9.430071
CH4	-8.100245	0.666680	0.670300	-2.271412
CN	-15.505811	0.272167	0.288800	-10.437318
CO	-21.747159	0.391502	0.413700	-13.929547
CO2	-37.870086	0.591351	0.621400	-18.855819
CS	-15.808673	0.254014	0.274000	-12.541678
Cl2	-30.004344	0.083838	0.094000	-6.376706
ClF	-39.275124	0.088509	0.100100	-7.273579
ClO	-30.979586	0.096255	0.104700	-5.299467
F2	-48.501355	0.048629	0.062200	-8.515754
H2CO	-22.936484	0.580334	0.596700	-10.269904
H2O	-17.275461	0.351890	0.371900	-12.556392
H2O2	-33.245379	0.398729	0.429400	-19.246046
H2S	-11.410104	0.287530	0.292000	-2.804710
H3COH	-24.153635	0.796992	0.818700	-13.621906
H3CSH	-18.296977	0.741331	0.757000	-9.832294
HCN	-16.217584	0.483693	0.496900	-8.287407
HCO	-22.285837	0.429934	0.444700	-9.266125
HCl	-15.625330	0.164831	0.171000	-3.871087
HF	-24.935022	0.208413	0.226100	-11.098820
HOCl	-31.628720	0.245143	0.264700	-12.272272
Li2	-0.432351	0.031357	0.038900	-4.733448
LiF	-24.637498	0.210638	0.222000	-7.129861
LiH	-0.795469	0.094726	0.092430	1.440471
N2	-19.950292	0.348162	0.364600	-10.315058
N2H4	-22.282112	0.678996	0.699600	-12.929499
NH	-10.439126	0.137814	0.133500	2.707283

2.6.3 $\mu = 0$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.995992				5
C	-5.415558				15
Cl	-14.940443				16
F	-24.189715				31
H	-0.500912				1
Li	-0.196167				1
N	-9.782786				29
Na	-0.181859				1
O	-15.894323				49
P	-6.462420				13
S	-10.109303				19
Si	-3.762540				9
BeH	-1.578351	0.081447	0.079400	1.284579	13
C2H2	-12.486658	0.653717	0.642400	7.101799	47
C2H4	-13.734919	0.900154	0.899000	0.724062	95
C2H6	-14.964457	1.127868	1.136900	-5.667860	191
CH	-6.048645	0.132174	0.133900	-1.082932	33
$CH2_{1A1}$	-6.697257	0.279875	0.288900	-5.663400	47
$CH2_{3B1}$	-6.720982	0.303599	0.304100	-0.314363	73
CH3	-7.404619	0.486325	0.490800	-2.808176	72
CH3Cl	-22.488560	0.629822	0.631000	-0.738983	191
CH4	-8.079908	0.660702	0.670300	-6.023073	95
CN	-15.505024	0.306679	0.288800	11.219545	84
CO	-21.732585	0.422703	0.413700	5.649403	95
CO2	-37.857754	0.653548	0.621400	20.173326	191
CS	-15.808316	0.283454	0.274000	5.932583	95
Cl2	-29.988360	0.107474	0.094000	8.455052	47
ClF	-39.243422	0.113264	0.100100	8.260677	95
ClO	-30.958747	0.123980	0.104700	12.098658	240
F2	-48.456767	0.077338	0.062200	9.498968	47
H2CO	-22.916997	0.605291	0.596700	5.390807	191
H2O	-17.252411	0.356263	0.371900	-9.812252	23
H2O2	-33.215957	0.425486	0.429400	-2.455895	191
H2S	-11.396005	0.284877	0.292000	-4.469499	23
H3COH	-24.124753	0.811223	0.818700	-4.691679	383
H3CSH	-18.278207	0.749697	0.757000	-4.582609	383
HCN	-16.210857	0.511600	0.496900	9.224172	95
HCO	-22.269427	0.458633	0.444700	8.743064	299
HCl	-15.608318	0.166963	0.171000	-2.532958	11
HF	-24.903995	0.213369	0.226100	-7.988970	47
HOCl	-31.605570	0.269892	0.264700	3.258070	191
Li2	-0.428677	0.036343	0.038900	-1.604381	5
LiF	-24.606297	0.220415	0.222000	-0.994505	23
LiH	-0.783411	0.086332	0.092430	-3.826415	5
N2	-19.943963	0.378390	0.364600	8.653352	47
N2H4	-22.260976	0.691755	0.699600	-4.922720	383
NH	-10.418508	0.134810	0.133500	0.821781	81

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		N
Be	-0.997691	0.000015	0.000000	0.000021				
C	-5.417028	0.000023	0.000000	0.000033				
Cl	-14.941519	0.000042	0.000000	0.000060				
F	-24.189637	0.000067	0.000000	0.000095				
H	-0.500002	0.000008	0.000000	0.000011				
Li	-0.196419	0.000002	0.000000	0.000003				
N	-9.789446	0.000116	0.000000	0.000164				
Na	-0.182142	0.000003	0.000000	0.000004				
O	-15.893331	0.000156	0.000000	0.000220				
P	-6.462465	0.000029	0.000000	0.000042				
S	-10.108990	0.000033	0.000000	0.000047				
Si	-3.758559	0.000026	0.000000	0.000037				
BeH	-1.587371	0.000685	0.089678	0.000685	0.079400	6.449530	0.430013	
C2H2	-12.491119	0.000143	0.657059	0.000151	0.642400	9.198847	0.094977	
C2H4	-13.744313	0.000153	0.910249	0.000163	0.899000	7.058664	0.102040	
C2H6	-14.985780	0.000267	1.151713	0.000275	1.136900	9.295102	0.172290	1
CH	-6.049921	0.000042	0.132891	0.000048	0.133900	-0.633032	0.030199	
$CH2_{1A1}$	-6.705087	0.000064	0.288055	0.000070	0.288900	-0.530061	0.044019	
$CH2_{3B1}$	-6.726587	0.000039	0.309555	0.000048	0.304100	3.423191	0.030193	
CH3	-7.414304	0.000072	0.497270	0.000079	0.490800	4.060166	0.049375	
CH3Cl	-22.492938	0.000675	0.634386	0.000677	0.631000	2.124594	0.425075	1
CH4	-8.094450	0.000070	0.677415	0.000080	0.670300	4.464655	0.050041	
CN	-15.488826	0.000099	0.282352	0.000154	0.288800	-4.046143	0.096917	
CO	-21.724654	0.000105	0.414295	0.000189	0.413700	0.373618	0.118741	
CO2	-37.830280	0.000259	0.626591	0.000406	0.621400	3.257186	0.254561	1
CS	-15.795598	0.000131	0.269580	0.000138	0.274000	-2.773893	0.086306	
Cl2	-29.976179	0.000188	0.093141	0.000206	0.094000	-0.538747	0.129335	
ClF	-39.225737	0.000248	0.094581	0.000260	0.100100	-3.463180	0.163182	
ClO	-30.932152	0.000271	0.097302	0.000315	0.104700	-4.642333	0.197734	2
F2	-48.426862	0.001154	0.047588	0.001161	0.062200	-9.169431	0.728730	
H2CO	-22.910378	0.000231	0.600016	0.000280	0.596700	2.080514	0.175622	1
H2O	-17.256879	0.000058	0.363544	0.000167	0.371900	-5.243288	0.104655	
H2O2	-33.198133	0.000311	0.411468	0.000440	0.429400	-11.252768	0.276385	1
H2S	-11.398220	0.000062	0.289227	0.000072	0.292000	-1.740360	0.045276	
H3COH	-24.131832	0.000446	0.821466	0.000474	0.818700	1.735401	0.297488	3
H3CSH	-18.285696	0.000340	0.759671	0.000344	0.757000	1.676056	0.215762	3
HCN	-16.206981	0.000106	0.500506	0.000159	0.496900	2.262684	0.099662	
HCO	-22.254871	0.000219	0.444511	0.000270	0.444700	-0.118796	0.169367	2
HCl	-15.611015	0.000052	0.169494	0.000067	0.171000	-0.944764	0.042175	
HF	-24.908333	0.000114	0.218694	0.000133	0.226100	-4.647615	0.083317	
HOCl	-31.591584	0.000264	0.256733	0.000310	0.264700	-4.999669	0.194331	1
Li2	-0.427761	0.000012	0.034924	0.000013	0.038900	-2.494725	0.007906	
LiF	-24.609167	0.000104	0.223111	0.000124	0.222000	0.697301	0.077810	
LiH	-0.788072	0.000014	0.091652	0.000016	0.092430	-0.488367	0.010340	
N2	-19.933846	0.000123	0.354955	0.000262	0.364600	-6.052491	0.164617	
N2H4	-22.262509	0.000229	0.683610	0.000327	0.699600	-10.033741	0.205384	3
NH	-10.418696	0.000055	0.129248	0.000129	0.133500	-2.667891	0.080786	

2.6.4 $\mu = 1/4$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.994638				13
C	-5.418798				18
Cl	-14.939612				127
F	-24.191803				31
H	-0.498892				1
Li	-0.198879				1
N	-9.787920				29
Na	-0.184562				1
O	-15.896821				42
P	-6.462610				61
S	-10.108434				122
Si	-3.760535				55
BeH	-1.580067	0.086537	0.079400	4.478799	13
C2H2	-12.488247	0.652867	0.642400	6.568077	740
C2H4	-13.737941	0.904777	0.899000	3.625083	904
C2H6	-14.971590	1.140641	1.136900	2.347662	6100
CH	-6.049247	0.131557	0.133900	-1.470090	66
$CH2_{1A1}$	-6.698159	0.281577	0.288900	-4.595339	171
$CH2_{3B1}$	-6.723904	0.307321	0.304100	2.021468	145
CH3	-7.407165	0.491690	0.490800	0.558782	162
CH3Cl	-22.488919	0.633833	0.631000	1.777928	7505
CH4	-8.082097	0.667731	0.670300	-1.612386	411
CN	-15.500503	0.293785	0.288800	3.128016	631
CO	-21.736860	0.421241	0.413700	4.731779	410
CO2	-37.860561	0.648121	0.621400	16.767976	1516
CS	-15.801669	0.274437	0.274000	0.274226	2396
Cl2	-29.982036	0.102812	0.094000	5.529465	2816
ClF	-39.243721	0.112307	0.100100	7.659794	795
ClO	-30.955604	0.119172	0.104700	9.081158	1948
F2	-48.459597	0.075991	0.062200	8.654136	90
H2CO	-22.920253	0.606850	0.596700	6.369094	763
H2O	-17.255917	0.361313	0.371900	-6.643652	47
H2O2	-33.221051	0.429625	0.429400	0.141428	673
H2S	-11.392667	0.286450	0.292000	-3.482939	337
H3COH	-24.132017	0.820830	0.818700	1.336494	3021
H3CSH	-18.278197	0.755397	0.757000	-1.005804	16693
HCN	-16.212193	0.506583	0.496900	6.076107	939
HCO	-22.272113	0.457603	0.444700	8.096455	1414
HCl	-15.606246	0.167743	0.171000	-2.044105	184
HF	-24.907592	0.216897	0.226100	-5.775072	46
HOCl	-31.605676	0.270351	0.264700	3.546025	1785
Li2	-0.427789	0.030031	0.038900	-5.565398	11
LiF	-24.612130	0.221448	0.222000	-0.346485	23
LiH	-0.785226	0.087455	0.092430	-3.122037	5
N2	-19.946137	0.370297	0.364600	3.574839	206
N2H4	-22.267523	0.696115	0.699600	-2.186674	10976
NH	-10.420498	0.133686	0.133500	0.116507	83

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		N
Be	-1.001590	0.000043	0.000000	0.000061				
C	-5.417927	0.000054	0.000000	0.000077				
Cl	-14.944713	0.000094	0.000000	0.000132				
F	-24.189771	0.000124	0.000000	0.000175				
H	-0.500003	0.000003	0.000000	0.000005				
Li	-0.196326	0.000001	0.000000	0.000002				
N	-9.789147	0.000096	0.000000	0.000136				
Na	-0.182144	0.000002	0.000000	0.000002				
O	-15.892839	0.000100	0.000000	0.000141				
P	-6.464868	0.000110	0.000000	0.000155				
S	-10.111848	0.000104	0.000000	0.000147				
Si	-3.760170	0.000093	0.000000	0.000131				
BeH	-1.587681	0.000968	0.086088	0.000969	0.079400	4.196953	0.608289	
C2H2	-12.494217	0.000740	0.658358	0.000748	0.642400	10.013558	0.469329	
C2H4	-13.746026	0.000731	0.910159	0.000739	0.899000	7.002674	0.463846	
C2H6	-14.985624	0.001553	1.149751	0.001557	1.136900	8.064219	0.977011	6
CH	-6.051869	0.000149	0.133939	0.000158	0.133900	0.024473	0.099450	
$CH2_{1A1}$	-6.707438	0.000168	0.289504	0.000177	0.288900	0.379233	0.110949	
$CH2_{3B1}$	-6.727000	0.000195	0.309066	0.000202	0.304100	3.116501	0.127051	
CH3	-7.414502	0.000267	0.496566	0.000273	0.490800	3.618093	0.171155	
CH3Cl	-22.497204	0.000814	0.634555	0.000821	0.631000	2.230530	0.515259	7
CH4	-8.094889	0.000260	0.676949	0.000266	0.670300	4.172378	0.166671	
CN	-15.493316	0.000323	0.286242	0.000342	0.288800	-1.605145	0.214493	
CO	-21.727277	0.000591	0.416512	0.000602	0.413700	1.764715	0.377752	
CO2	-37.834494	0.001061	0.630891	0.001081	0.621400	5.955412	0.678100	1
CS	-15.801754	0.000473	0.271980	0.000487	0.274000	-1.267778	0.305696	2
Cl2	-29.983444	0.000262	0.094019	0.000322	0.094000	0.011860	0.202027	2
ClF	-39.230571	0.001266	0.096087	0.001275	0.100100	-2.518353	0.800330	
ClO	-30.938412	0.001326	0.100861	0.001333	0.104700	-2.409223	0.836426	1
F2	-48.427172	0.001422	0.047629	0.001443	0.062200	-9.143526	0.905584	
H2CO	-22.912668	0.000971	0.601896	0.000978	0.596700	3.260448	0.613736	
H2O	-17.256742	0.000138	0.363897	0.000170	0.371900	-5.021915	0.106972	
H2O2	-33.198202	0.001182	0.412518	0.001199	0.429400	-10.593674	0.752184	
H2S	-11.401024	0.000473	0.289170	0.000485	0.292000	-1.775791	0.304069	
H3COH	-24.134729	0.001455	0.823950	0.001459	0.818700	3.294480	0.915545	3
H3CSH	-18.292972	0.003027	0.763185	0.003029	0.757000	3.881053	1.900931	16
HCN	-16.209478	0.000514	0.502401	0.000525	0.496900	3.451700	0.329653	
HCO	-22.258099	0.001179	0.447330	0.001185	0.444700	1.650410	0.743419	1
HCl	-15.614199	0.000231	0.169483	0.000249	0.171000	-0.951770	0.156484	
HF	-24.908326	0.000208	0.218551	0.000242	0.226100	-4.737052	0.151753	
HOCl	-31.595232	0.000915	0.257677	0.000925	0.264700	-4.406973	0.580448	1
Li2	-0.430590	0.000038	0.037938	0.000038	0.038900	-0.603381	0.023999	
LiF	-24.609057	0.000282	0.222960	0.000308	0.222000	0.602284	0.193372	
LiH	-0.788100	0.000043	0.091771	0.000043	0.092430	-0.413476	0.027256	
N2	-19.936311	0.000241	0.358017	0.000309	0.364600	-4.130596	0.193700	
N2H4	-22.258558	0.003514	0.680251	0.003519	0.699600	-12.141860	2.208304	10
NH	-10.419077	0.000161	0.129926	0.000187	0.133500	-2.242480	0.117556	

2.6.5 $\mu = 1/2$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.998262				11
C	-5.426287				142
Cl	-14.945871				1745
F	-24.216187				332
H	-0.502296				1
Li	-0.196739				1
N	-9.802906				278
Na	-0.182371				1
O	-15.914975				369
P	-6.465047				659
S	-10.111838				1094
Si	-3.759602				273
BeH	-1.582425	0.081867	0.079400	1.547929	141
C2H2	-12.491868	0.634701	0.642400	-4.831432	24583
C2H4	-13.744979	0.883220	0.899000	-9.902176	48984
C2H6	-14.984867	1.118515	1.136900	-11.536821	387245
CH	-6.054906	0.126323	0.133900	-4.754955	1207
$CH2_{1A1}$	-6.704228	0.273349	0.288900	-9.758615	1463
$CH2_{3B1}$	-6.732656	0.301776	0.304100	-1.458423	2609
CH3	-7.415705	0.482530	0.490800	-5.189750	3357
CH3Cl	-22.496886	0.617839	0.631000	-8.258935	401797
CH4	-8.091636	0.656164	0.670300	-8.870454	27417
CN	-15.500623	0.271430	0.288800	-10.899857	22915
CO	-21.746748	0.405486	0.413700	-5.154533	10430
CO2	-37.874991	0.618753	0.621400	-1.660920	92560
CS	-15.799741	0.261616	0.274000	-7.771368	149631
Cl2	-29.984427	0.092684	0.094000	-0.825724	188008
ClF	-39.259993	0.097935	0.100100	-1.358376	46952
ClO	-30.961899	0.101053	0.104700	-2.288617	87113
F2	-48.486273	0.053899	0.062200	-5.208688	8432
H2CO	-22.931847	0.585993	0.596700	-6.719052	43317
H2O	-17.271322	0.351755	0.371900	-12.641249	1685
H2O2	-33.239150	0.404607	0.429400	-15.557645	91645
H2S	-11.395645	0.279215	0.292000	-8.022687	5996
H3COH	-24.150723	0.800276	0.818700	-11.561197	145275
H3CSH	-18.285085	0.737775	0.757000	-12.063768	1661290
HCN	-16.216291	0.484802	0.496900	-7.591671	37520
HCO	-22.281172	0.437613	0.444700	-4.447041	103416
HCl	-15.611645	0.163478	0.171000	-4.720164	6332
HF	-24.930165	0.211682	0.226100	-9.047528	1228
HOCl	-31.616075	0.252932	0.264700	-7.384381	97849
Li2	-0.429005	0.035528	0.038900	-2.116218	11
LiF	-24.633580	0.220654	0.222000	-0.844350	881
LiH	-0.785530	0.086495	0.092430	-3.724376	11
N2	-19.952279	0.346468	0.364600	-11.377891	8914
N2H4	-22.281405	0.666410	0.699600	-20.827273	202086
NH	-10.431265	0.126064	0.133500	-4.666383	1194

2. DMC without Jastrow

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
Be	-1.007273	0.000009					
C	-5.422968	0.000059					
Cl	-14.953296	0.000209					
F	-24.191160	0.000154					
H	-0.500003	0.000003					
Li	-0.196326	0.000001					
N	-9.791066	0.000107					
Na	-0.182144	0.000002					
O	-15.894932	0.000153					
P	-6.470170	0.000104					
S	-10.118934	0.000134					
Si	-3.763979	0.000054					
C2H2	-12.494688	0.001235	0.648746	0.001241	0.642400	3.982276	0.778450
C2H4	-13.747089	0.000912	0.901140	0.000920	0.899000	1.343007	0.577336
C2H6	-14.985170	0.001895	1.139215	0.001899	1.136900	1.452418	1.191346
CH	-6.056925	0.000143	0.133954	0.000155	0.133900	0.033677	0.097047
$CH2_{1A1}$	-6.712542	0.000231	0.289567	0.000239	0.288900	0.418832	0.149699
$CH2_{3B1}$	-6.728932	0.000180	0.305958	0.000190	0.304100	1.165904	0.118975
CH3	-7.415797	0.000290	0.492820	0.000296	0.490800	1.267433	0.185621
CH3Cl	-22.505354	0.001446	0.629080	0.001463	0.631000	-1.204557	0.917741
CH4	-8.096248	0.000660	0.673268	0.000663	0.670300	1.862189	0.416055
CN	-15.503306	0.000713	0.289272	0.000724	0.288800	0.296287	0.454036
CO	-21.733058	0.000647	0.415158	0.000667	0.413700	0.915093	0.418591
CO2	-37.835639	0.001461	0.622807	0.001494	0.621400	0.882948	0.937235
CS	-15.813849	0.001321	0.271948	0.001329	0.274000	-1.287607	0.833910
Cl2	-29.999495	0.000811	0.092903	0.000912	0.094000	-0.688477	0.572592
ClF	-39.240347	0.001286	0.095891	0.001312	0.100100	-2.641149	0.823116
ClO	-30.948563	0.000697	0.100335	0.000744	0.104700	-2.739001	0.466689
F2	-48.436023	0.001138	0.053704	0.001179	0.062200	-5.331380	0.740021
H2CO	-22.915040	0.001390	0.597134	0.001400	0.596700	0.272229	0.878441
H2O	-17.257413	0.000339	0.362474	0.000372	0.371900	-5.914913	0.233416
H2O2	-33.203269	0.001407	0.413398	0.001439	0.429400	-10.041147	0.903240
H2S	-11.408073	0.000327	0.289133	0.000354	0.292000	-1.799156	0.221884
H3COH	-24.131302	0.001079	0.813389	0.001091	0.818700	-3.332420	0.684594
H3CSH	-18.295769	0.002132	0.753855	0.002137	0.757000	-1.973515	1.340994
HCN	-16.215590	0.000516	0.501553	0.000530	0.496900	2.919772	0.332894
HCO	-22.262855	0.000653	0.444952	0.000673	0.444700	0.157981	0.422590
HCl	-15.623938	0.000347	0.170638	0.000405	0.171000	-0.226874	0.254259
HF	-24.909404	0.000297	0.218241	0.000335	0.226100	-4.931461	0.209988
HOCl	-31.605993	0.002131	0.257761	0.002147	0.264700	-4.354028	1.346990
Li2	-0.431440	0.000008	0.038788	0.000008	0.038900	-0.070155	0.005267
LiF	-24.610538	0.000294	0.223053	0.000332	0.222000	0.660455	0.208127
LiH	-0.788315	0.000019	0.091986	0.000020	0.092430	-0.278642	0.012388
N2	-19.943693	0.000729	0.361561	0.000760	0.364600	-1.907298	0.477133
N2H4	-22.265700	0.000962	0.683554	0.000986	0.699600	-10.068869	0.618588
NH	-10.420721	0.000217	0.129651	0.000242	0.133500	-2.415160	0.152002
NH2	-11.077790	0.000288	0.286717	0.000307	0.290400	-2.310806	0.192766

3. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.007279	0.000010						
C	-5.423300	0.000028						
Cl	-14.952683	0.000062						
F	-24.190436	0.000075						
H	-0.499985	0.000011						
Li	-0.196399	0.000005						
N	-9.790924	0.000035						
Na	-0.182137	0.000007						
O	-15.894747	0.000067						
P	-6.470037	0.000035						
S	-10.119025	0.000035						
Si	-3.763903	0.000028						
BeH	-1.588032	0.000589	0.080752	0.000589	0.079400	0.848293	0.369822	
C2H2	-12.496830	0.000139	0.650259	0.000151	0.642400	4.931311	0.094797	
C2H4	-13.748335	0.000253	0.901793	0.000263	0.899000	1.752944	0.165097	
C2H6	-14.985987	0.000354	1.139475	0.000364	1.136900	1.616022	0.228669	3
CH	-6.057005	0.000034	0.133720	0.000045	0.133900	-0.113147	0.028276	
$CH2_{1A1}$	-6.712121	0.000156	0.288850	0.000160	0.288900	-0.031542	0.100246	
$CH2_{3B1}$	-6.728900	0.000059	0.305629	0.000069	0.304100	0.959761	0.043049	
CH3	-7.415471	0.000072	0.492215	0.000084	0.490800	0.888074	0.052768	
CH3Cl	-22.505299	0.000372	0.629360	0.000380	0.631000	-1.029174	0.238397	4
CH4	-8.094962	0.000117	0.671721	0.000128	0.670300	0.891799	0.080400	
CN	-15.501002	0.000128	0.286778	0.000135	0.288800	-1.268868	0.085020	
CO	-21.732238	0.000207	0.414190	0.000220	0.413700	0.307489	0.137747	
CO2	-37.834814	0.000405	0.622019	0.000427	0.621400	0.388267	0.268207	
CS	-15.813266	0.000148	0.270940	0.000154	0.274000	-1.920002	0.096742	1
Cl2	-29.998521	0.000254	0.093154	0.000283	0.094000	-0.530997	0.177333	1
ClF	-39.237751	0.000529	0.094632	0.000538	0.100100	-3.431508	0.337383	
ClO	-30.946811	0.000668	0.099381	0.000675	0.104700	-3.337889	0.423311	
F2	-48.431519	0.000442	0.050646	0.000466	0.062200	-7.250132	0.292662	
H2CO	-22.914978	0.000451	0.596960	0.000457	0.596700	0.163005	0.286691	
H2O	-17.256930	0.000133	0.362213	0.000150	0.371900	-6.078877	0.094134	
H2O2	-33.202255	0.000303	0.412790	0.000332	0.429400	-10.422696	0.208441	
H2S	-11.408279	0.000096	0.289284	0.000105	0.292000	-1.704594	0.065613	
H3COH	-24.131103	0.000308	0.813114	0.000320	0.818700	-3.505144	0.200689	1
H3CSH	-18.294959	0.000174	0.752693	0.000185	0.757000	-2.702788	0.116026	16
HCN	-16.213835	0.000178	0.499625	0.000183	0.496900	1.710061	0.115079	
HCO	-22.261112	0.000252	0.443079	0.000262	0.444700	-1.017257	0.164520	1
HCl	-15.622819	0.000098	0.170150	0.000117	0.171000	-0.533467	0.073175	
HF	-24.907600	0.000195	0.217179	0.000209	0.226100	-5.598263	0.131401	
HOCl	-31.604134	0.000421	0.256718	0.000431	0.264700	-5.008728	0.270249	
Li2	-0.431447	0.000021	0.038648	0.000024	0.038900	-0.157824	0.014916	
LiF	-24.608673	0.000148	0.221837	0.000166	0.222000	-0.102139	0.104155	
LiH	-0.788327	0.000040	0.091942	0.000041	0.092430	-0.306019	0.026010	
N2	-19.941389	0.000208	0.359541	0.000219	0.364600	-3.174437	0.137387	
N2H4	-22.263237	0.000279	0.681449	0.000291	0.699600	-11.390179	0.182758	2
NH	-10.420457	0.000137	0.129548	0.000142	0.133500	-2.479749	0.088842	

2.6.6 $\mu = 1$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-1.004590				10
C	-5.426316				595
Cl	-14.950775				14342
F	-24.226718				2075
H	-0.500912				1
Li	-0.196167				1
N	-9.805482				1010
Na	-0.181859				1
O	-15.916920				2197
P	-6.468202				2442
S	-10.115949				10386
Si	-3.761555				1077
BeH	-1.581295	0.075793	0.079400	-2.263666	433
C2H2	-12.488261	0.633806	0.642400	-5.392909	1724878
C2H4	-13.740253	0.883973	0.899000	-9.429309	10195715
C2H6	-14.974869	1.116766	1.136900	-12.634429	1342000
CH	-6.054007	0.126780	0.133900	-4.468142	8664
$CH2_{1A1}$	-6.704677	0.276538	0.288900	-7.757554	21073
$CH2_{3B1}$	-6.729974	0.301834	0.304100	-1.421740	17180
CH3	-7.412471	0.483419	0.490800	-4.631504	53073
CH3Cl	-22.496305	0.616478	0.631000	-9.112655	12059155
CH4	-8.089555	0.659591	0.670300	-6.719762	586258
CN	-15.498796	0.266998	0.288800	-13.681140	2339948
CO	-21.742030	0.398794	0.413700	-9.353728	825873
CO2	-37.863440	0.603285	0.621400	-11.367516	10551823
CS	-15.804672	0.262407	0.274000	-7.274581	12788080
Cl2	-29.989661	0.088111	0.094000	-3.695499	12649041
ClF	-39.264756	0.087263	0.100100	-8.055144	6058905
ClO	-30.958888	0.091193	0.104700	-8.475641	10688267
F2	-48.490135	0.036699	0.062200	-16.002263	402515
H2CO	-22.924975	0.579915	0.596700	-10.532790	6396819
H2O	-17.270606	0.351863	0.371900	-12.573679	25915
H2O2	-33.229068	0.393404	0.429400	-22.587767	13264605
H2S	-11.400389	0.282617	0.292000	-5.888208	201179
H3COH	-24.143007	0.796123	0.818700	-14.167006	13019016
H3CSH	-18.273976	0.728063	0.757000	-18.158141	1329615
HCN	-16.210057	0.477347	0.496900	-12.269523	1516119
HCO	-22.273743	0.429595	0.444700	-9.478440	11299202
HCl	-15.617871	0.166184	0.171000	-3.021801	104095
HF	-24.938806	0.211175	0.226100	-9.365274	10957
HOCl	-31.614009	0.245402	0.264700	-12.109566	13009384
Li2	-0.430399	0.038065	0.038900	-0.523966	44
LiF	-24.638816	0.215931	0.222000	-3.808194	13044
LiH	-0.784321	0.087243	0.092430	-3.255145	41
N2	-19.943468	0.332504	0.364600	-20.140693	788381
N2H4	-22.267946	0.653334	0.699600	-29.032225	13887352

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.009333	0.000023	0.000000	0.000032				
C	-5.429952	0.000254	0.000000	0.000360				
Cl	-14.966696	0.000236	0.000000	0.000334				
F	-24.189361	0.000258	0.000000	0.000365				
H	-0.500004	0.000003	0.000000	0.000005				
Li	-0.196327	0.000001	0.000000	0.000002				
N	-9.796123	0.000634	0.000000	0.000896				
Na	-0.182143	0.000002	0.000000	0.000003				
O	-15.897308	0.000167	0.000000	0.000236				
P	-6.474481	0.000451	0.000000	0.000638				
S	-10.128988	0.000160	0.000000	0.000226				
Si	-3.766828	0.000191	0.000000	0.000270				
BeH	-1.587760	0.000404	0.078422	0.000405	0.079400	-0.613625	0.254225	
C2H2	-12.501205	0.000477	0.641292	0.000697	0.642400	-0.695563	0.437438	1
C2H4	-13.752980	0.001163	0.893057	0.001269	0.899000	-3.729083	0.796528	10
C2H6	-14.986407	0.001131	1.126476	0.001240	1.136900	-6.541293	0.778411	1
CH	-6.063568	0.000138	0.133611	0.000289	0.133900	-0.181404	0.181661	
$CH2_{1A1}$	-6.717705	0.000218	0.287744	0.000335	0.288900	-0.725514	0.210234	
$CH2_{3B1}$	-6.731842	0.000180	0.301881	0.000312	0.304100	-1.392327	0.195630	
CH3	-7.417017	0.000286	0.487052	0.000383	0.490800	-2.352058	0.240377	
CH3Cl	-22.512367	0.003390	0.615706	0.003407	0.631000	-9.597160	2.138213	12
CH4	-8.095743	0.000843	0.665773	0.000881	0.670300	-2.840799	0.552812	
CN	-15.509921	0.002042	0.283845	0.002153	0.288800	-3.109134	1.351245	2
CO	-21.736593	0.002474	0.409333	0.002493	0.413700	-2.740306	1.564333	
CO2	-37.834149	0.001030	0.609581	0.001112	0.621400	-7.416365	0.697814	10
CS	-15.829831	0.001401	0.270891	0.001432	0.274000	-1.951220	0.898880	12
Cl2	-30.018175	0.001747	0.084783	0.001810	0.094000	-5.783619	1.135684	12
ClF	-39.255045	0.003115	0.098988	0.003134	0.100100	-0.697741	1.966796	6
ClO	-30.958774	0.001094	0.094771	0.001131	0.104700	-6.230738	0.709881	10
F2	-48.423955	0.001149	0.045233	0.001259	0.062200	-10.646862	0.790293	
H2CO	-22.914273	0.002474	0.587004	0.002493	0.596700	-6.084427	1.564160	6
H2O	-17.257799	0.000249	0.360482	0.000300	0.371900	-7.164861	0.188259	
H2O2	-33.201854	0.001451	0.407229	0.001489	0.429400	-13.912448	0.934071	13
H2S	-11.416652	0.000452	0.287655	0.000480	0.292000	-2.726256	0.300976	
H3COH	-24.100072	0.001474	0.772794	0.001505	0.818700	-28.806168	0.944554	13
H3CSH	-18.301426	0.001376	0.742468	0.001409	0.757000	-9.118962	0.884061	1
HCN	-16.222226	0.002577	0.496146	0.002666	0.496900	-0.473224	1.672950	1
HCO	-22.262605	0.002012	0.435340	0.002035	0.444700	-5.873355	1.277162	11
HCl	-15.635528	0.000529	0.168828	0.000580	0.171000	-1.362840	0.363821	
HF	-24.906637	0.000675	0.217271	0.000723	0.226100	-5.540270	0.453406	
HOCl	-31.612011	0.001290	0.248003	0.001322	0.264700	-10.477520	0.829696	13
Li2	-0.431540	0.000021	0.038886	0.000021	0.038900	-0.008849	0.012984	
LiF	-24.605932	0.000703	0.220244	0.000748	0.222000	-1.101968	0.469642	
LiH	-0.788442	0.000037	0.092110	0.000037	0.092430	-0.200593	0.023276	
N2	-19.949860	0.000510	0.357614	0.001366	0.364600	-4.383977	0.857123	
N2H4	-22.272664	0.001553	0.680400	0.002005	0.699600	-12.048205	1.257986	13
NH	-10.425105	0.000181	0.128977	0.000659	0.133500	-2.837971	0.413506	

2.6.7 FCI

1. CIPSI

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
	e_{cal}	ae_{cal}	ae_{nr}	ae_{diff}	Ndet		
Be	-1.008492	0.000096	0.000000	0.000136			
C	-5.428008	0.000013	0.000000	0.000018			
Cl	-14.946282	0.000006	0.000000	0.000008			
F	-24.163567	0.000015	0.000000	0.000022			
H	-0.499043	0.000000		0.000000			
Li	-0.196093	0.000000		0.000000			
N	-9.790978	0.000017	0.000000	0.000024			
Na	-0.181799	0.000000		0.000000			
O	-15.882573	0.000003	0.000000	0.000005			
P	-6.469736	0.000011	0.000000	0.000016			
S	-10.116024	0.000004	0.000000	0.000005			
Si	-3.763624	0.000004	0.000000	0.000006			
BeH	-1.581896	0.000006	0.074361	0.000096	0.079400	-3.161966	0.060369
C2H2	-12.480026	0.000012	0.625924	0.000029	0.642400	-10.338930	0.018082
C2H4	-13.728870	0.000006	0.876682	0.000027	0.899000	-14.004549	0.016869
C2H6	-14.962048	0.000071	1.111774	0.000075	1.136900	-15.766666	0.047243
CH	-6.056891	0.000012	0.129840	0.000018	0.133900	-2.547402	0.011185
$CH2_{1A1}$	-6.707051	0.000001	0.280957	0.000013	0.288900	-4.984375	0.008216
$CH2_{3B1}$	-6.722856	0.000001	0.296762	0.000013	0.304100	-4.604681	0.008211
CH3	-7.405038	0.000003	0.479901	0.000013	0.490800	-6.839150	0.008352
CH3Cl	-22.482202	0.000192	0.610783	0.000192	0.631000	-12.686100	0.120698
CH4	-8.081441	0.000003	0.657261	0.000013	0.670300	-8.182009	0.008369
CN	-15.492696	0.000012	0.273709	0.000025	0.288800	-9.469446	0.015446
CO	-21.711419	0.000010	0.400838	0.000017	0.413700	-8.070933	0.010478
CO2	-37.789127	0.000280	0.595973	0.000280	0.621400	-15.955684	0.175794
CS	-15.804633	0.000026	0.260602	0.000029	0.274000	-8.407530	0.018250
Cl2	-29.976481	0.000134	0.083918	0.000134	0.094000	-6.326863	0.084129
ClF	-39.198263	0.000065	0.088414	0.000067	0.100100	-7.333314	0.042078
ClO	-30.920322	0.000119	0.091467	0.000119	0.104700	-8.303758	0.074797
F2	-48.381050	0.000011	0.053916	0.000033	0.062200	-5.198481	0.020403
H2CO	-22.886870	0.000011	0.578203	0.000018	0.596700	-11.607272	0.011035
H2O	-17.232161	0.000002	0.351502	0.000004	0.371900	-12.799685	0.002568
H2O2	-33.162975	0.000103	0.399743	0.000103	0.429400	-18.610108	0.064945
H2S	-11.396719	0.000001	0.282610	0.000004	0.292000	-5.892275	0.002478
H3COH	-24.097503	0.000398	0.790750	0.000399	0.818700	-17.539036	0.250143
H3CSH	-18.272893	0.000166	0.732690	0.000167	0.757000	-15.254781	0.104485
HCN	-16.197340	0.000001	0.479311	0.000021	0.496900	-11.037336	0.013463
HCO	-22.237063	0.000102	0.427439	0.000103	0.444700	-10.831638	0.064768
HCl	-15.610478	0.000005	0.165154	0.000008	0.171000	-3.668681	0.004717
HF	-24.874009	0.000000	0.211399	0.000015	0.226100	-9.225112	0.009632
HOCl	-31.572985	0.000036	0.245087	0.000037	0.264700	-12.307511	0.023157
Li2	-0.431306	0.000048	0.039119	0.000048	0.038900	0.137726	0.029851
LiF	-24.572038	0.000009	0.212377	0.000018	0.222000	-6.038485	0.011269
LiH	-0.786051	0.000034	0.090914	0.000034	0.092430	-0.951129	0.021442
N2	-19.925579	0.000008	0.343623	0.000035	0.364600	-13.163277	0.021925

2.7 VQZ-BFD

2.7.1 CCSD(T)

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-1.009630			
C	-5.431625			
Cl	-14.966606			
F	-24.185858			
H	-0.499916			
Li	-0.196307			
N	-9.798032			
Na	-0.181980			
O	-15.897220			
P	-6.475063			
S	-10.127554			
Si	-3.766083			
BeH	-1.588693	0.079148	0.079400	-0.158381
C2H2	-12.497962	0.634880	0.642400	-4.718627
C2H4	-13.748624	0.885711	0.899000	-8.338980
C2H6	-14.983956	1.121211	1.136900	-9.844858
CH	-6.063322	0.131782	0.133900	-1.329284
$CH2_{1A1}$	-6.715727	0.284271	0.288900	-2.905053
$CH2_{3B1}$	-6.730719	0.299262	0.304100	-3.035889
CH3	-7.415146	0.483774	0.490800	-4.409049
CH3Cl	-22.517441	0.619462	0.631000	-7.240005
CH4	-8.093188	0.661900	0.670300	-5.271213
CN	-15.508665	0.279009	0.288800	-6.143988
CO	-21.737434	0.408590	0.413700	-3.206882
CO2	-37.835937	0.609872	0.621400	-7.233662
CS	-15.827248	0.268069	0.274000	-3.721846
Cl2	-30.024045	0.090834	0.094000	-1.986971
ClF	-39.248024	0.095561	0.100100	-2.848329
ClO	-30.962404	0.098578	0.104700	-3.841333
F2	-48.429318	0.057603	0.062200	-2.884515
H2CO	-22.915905	0.587228	0.596700	-5.943614
H2O	-17.255568	0.358516	0.371900	-8.398330
H2O2	-33.205024	0.410751	0.429400	-11.702127
H2S	-11.415620	0.288234	0.292000	-2.363501
H3COH	-24.130100	0.801592	0.818700	-10.735687
H3CSH	-18.302410	0.743567	0.757000	-8.429457
HCN	-16.218749	0.489177	0.496900	-4.846491
HCO	-22.263922	0.435162	0.444700	-5.985318
HCl	-15.635201	0.168679	0.171000	-1.456303
HF	-24.901984	0.216210	0.226100	-6.205772
HOCl	-31.618416	0.254674	0.264700	-6.291255
Li2	-0.431450	0.038836	0.038900	-0.040420
LiF	-24.599303	0.217138	0.222000	-3.050674
LiH	-0.787778	0.091555	0.092430	-0.549226

2.7.2 DFT

1. PBE

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.996113			
C	-5.419470			
Cl	-14.944710			
F	-24.193963			
H	-0.499094			
Li	-0.200892			
N	-9.787765			
Na	-0.187644			
O	-15.900388			
P	-6.463886			
S	-10.113756			
Si	-3.765284			
BeH	-1.585461	0.090254	0.079400	6.810859
C2H2	-12.488592	0.651463	0.642400	5.686932
C2H4	-13.736782	0.901463	0.899000	1.545791
C2H6	-14.966450	1.132943	1.136900	-2.483005
CH	-6.052660	0.134095	0.133900	0.122198
$CH2_{1A1}$	-6.698745	0.281086	0.288900	-4.903179
$CH2_{3B1}$	-6.729359	0.311700	0.304100	4.768983
CH3	-7.409139	0.492385	0.490800	0.994623
CH3Cl	-22.491130	0.629667	0.631000	-0.836418
CH4	-8.080418	0.664570	0.670300	-3.595759
CN	-15.511957	0.304722	0.288800	9.991015
CO	-21.735759	0.415900	0.413700	1.380417
CO2	-37.861779	0.641531	0.621400	12.632694
CS	-15.811579	0.278352	0.274000	2.731125
Cl2	-29.992204	0.102785	0.094000	5.512432
ClF	-39.248033	0.109360	0.100100	5.811056
ClO	-30.967368	0.122270	0.104700	11.025649
F2	-48.459866	0.071941	0.062200	6.112297
H2CO	-22.920021	0.601974	0.596700	3.309249
H2O	-17.255624	0.357046	0.371900	-9.320794
H2O2	-33.220408	0.421442	0.429400	-4.993414
H2S	-11.398268	0.286323	0.292000	-3.562416
H3COH	-24.127495	0.811259	0.818700	-4.669484
H3CSH	-18.282355	0.752751	0.757000	-2.666170
HCN	-16.213545	0.507216	0.496900	6.473084
HCO	-22.275067	0.456114	0.444700	7.162174
HCl	-15.610589	0.166785	0.171000	-2.645028
HF	-24.907159	0.214102	0.226100	-7.528823
HOCl	-31.610199	0.266007	0.264700	0.820118
Li2	-0.428778	0.026993	0.038900	-7.471700
LiF	-24.608982	0.214127	0.222000	-4.940238
LiH	-0.783966	0.083979	0.092430	-5.303148
N2	-19.947513	0.371984	0.364600	4.633387
N2H4	-22.264991	0.693084	0.699600	-4.088952
NH	-10.425731	0.138871	0.133500	3.370565

2. BLYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.991021			
C	-5.412598			
Cl	-14.919841			
F	-24.196641			
H	-0.496668			
Li	-0.196523			
N	-9.774215			
Na	-0.183513			
O	-15.896302			
P	-6.436362			
S	-10.088113			
Si	-3.746117			
BeH	-1.581105	0.093416	0.079400	8.794900
C2H2	-12.444933	0.626402	0.642400	-10.039185
C2H4	-13.685815	0.873948	0.899000	-15.720380
C2H6	-14.907022	1.101818	1.136900	-22.014161
CH	-6.043997	0.134732	0.133900	0.521937
$CH2_{1A1}$	-6.687178	0.281244	0.288900	-4.804164
$CH2_{3B1}$	-6.706316	0.300382	0.304100	-2.333016
CH3	-7.385337	0.482736	0.490800	-5.060413
CH3Cl	-22.429883	0.607440	0.631000	-14.784249
CH4	-8.052982	0.653713	0.670300	-10.408709
CN	-15.475762	0.288949	0.288800	0.093706
CO	-21.708370	0.399470	0.413700	-8.929264
CO2	-37.811066	0.605864	0.621400	-9.748869
CS	-15.763990	0.263279	0.274000	-6.727259
Cl2	-29.928995	0.089312	0.094000	-2.941646
ClF	-39.215763	0.099281	0.100100	-0.514109
ClO	-30.926204	0.110061	0.104700	3.364026
F2	-48.459108	0.065827	0.062200	2.275710
H2CO	-22.884610	0.582374	0.596700	-8.989620
H2O	-17.241272	0.351634	0.371900	-12.717165
H2O2	-33.194243	0.408302	0.429400	-13.238958
H2S	-11.365291	0.283842	0.292000	-5.119299
H3COH	-24.084315	0.788744	0.818700	-18.797902
H3CSH	-18.217455	0.730072	0.757000	-16.897596
HCN	-16.175282	0.491801	0.496900	-3.199774
HCO	-22.242930	0.437362	0.444700	-4.604523
HCl	-15.579836	0.163327	0.171000	-4.814990
HF	-24.903739	0.210430	0.226100	-9.832805
HOCl	-31.565360	0.252548	0.264700	-7.625330
Li2	-0.423060	0.030014	0.038900	-5.575805
LiF	-24.608480	0.215317	0.222000	-4.193856
LiH	-0.786232	0.093041	0.092430	0.383328
N2	-19.912735	0.364304	0.364600	-0.185701
N2H4	-22.214434	0.679331	0.699600	-12.718722
NH	-10.410820	0.139936	0.133500	4.038817

3. PBE0

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.997452			
C	-5.422029			
Cl	-14.950878			
F	-24.192415			
H	-0.500774			
Li	-0.201291			
N	-9.792066			
Na	-0.187727			
O	-15.900799			
P	-6.467975			
S	-10.118676			
Si	-3.766609			
BeH	-1.588594	0.090369	0.079400	6.883073
C2H2	-12.485145	0.639540	0.642400	-1.794676
C2H4	-13.740661	0.893509	0.899000	-3.445750
C2H6	-14.978721	1.130021	1.136900	-4.316348
CH	-6.054538	0.131735	0.133900	-1.358557
$CH2_{1A1}$	-6.701849	0.278273	0.288900	-6.668662
$CH2_{3B1}$	-6.734346	0.310770	0.304100	4.185512
CH3	-7.415620	0.491270	0.490800	0.295188
CH3Cl	-22.499556	0.624328	0.631000	-4.186577
CH4	-8.088442	0.663318	0.670300	-4.381238
CN	-15.493699	0.279605	0.288800	-5.769987
CO	-21.722253	0.399425	0.413700	-8.957910
CO2	-37.833733	0.610105	0.621400	-7.087414
CS	-15.803592	0.262888	0.274000	-6.972920
Cl2	-29.995791	0.094036	0.094000	0.022690
ClF	-39.236734	0.093441	0.100100	-4.178380
ClO	-30.954652	0.102975	0.104700	-1.082362
F2	-48.430335	0.045504	0.062200	-10.476798
H2CO	-22.909527	0.585152	0.596700	-7.246535
H2O	-17.250915	0.348568	0.371900	-14.640869
H2O2	-33.199395	0.396249	0.429400	-20.802315
H2S	-11.403814	0.283591	0.292000	-5.276874
H3COH	-24.125892	0.799969	0.818700	-11.754054
H3CSH	-18.291108	0.747309	0.757000	-6.081038
HCN	-16.202675	0.487807	0.496900	-5.706188
HCO	-22.260629	0.437027	0.444700	-4.814763
HCl	-15.616600	0.164948	0.171000	-3.797412
HF	-24.901005	0.207816	0.226100	-11.473292
HOCl	-31.601767	0.249317	0.264700	-9.653257
Li2	-0.429768	0.027186	0.038900	-7.350531
LiF	-24.598395	0.204688	0.222000	-10.863154
LiH	-0.785007	0.082943	0.092430	-5.953161
N2	-19.932145	0.348013	0.364600	-10.408226
N2H4	-22.261313	0.674087	0.699600	-16.009406
NH	-10.427051	0.134212	0.133500	0.446761

4. B3LYP

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-1.001255			
C	-5.432926			
Cl	-14.960683			
F	-24.226982			
H	-0.501546			
Li	-0.200648			
N	-9.801448			
Na	-0.187270			
O	-15.923588			
P	-6.464937			
S	-10.122374			
Si	-3.766700			
BeH	-1.596944	0.094142	0.079400	9.250975
C2H2	-12.496314	0.627370	0.642400	-9.431554
C2H4	-13.753737	0.881700	0.899000	-10.856141
C2H6	-14.992301	1.117171	1.136900	-12.379953
CH	-6.069189	0.134717	0.133900	0.512485
$CH2_{1A1}$	-6.719706	0.283687	0.288900	-3.271109
$CH2_{3B1}$	-6.739885	0.303866	0.304100	-0.146864
CH3	-7.425926	0.488361	0.490800	-1.530256
CH3Cl	-22.512309	0.614061	0.631000	-10.629428
CH4	-8.101321	0.662210	0.670300	-5.076642
CN	-15.508332	0.273958	0.288800	-9.313486
CO	-21.750271	0.393758	0.413700	-12.514055
CO2	-37.874378	0.594277	0.621400	-17.019776
CS	-15.811994	0.256694	0.274000	-10.859752
Cl2	-30.007877	0.086511	0.094000	-4.699652
ClF	-39.279276	0.091611	0.100100	-5.327128
ClO	-30.983992	0.099721	0.104700	-3.124255
F2	-48.503861	0.049897	0.062200	-7.720035
H2CO	-22.939619	0.580012	0.596700	-10.471684
H2O	-17.278376	0.351695	0.371900	-12.678768
H2O2	-33.249734	0.399465	0.429400	-18.784350
H2S	-11.412149	0.286682	0.292000	-3.337173
H3COH	-24.157150	0.794451	0.818700	-15.216770
H3CSH	-18.300357	0.738872	0.757000	-11.375799
HCN	-16.220379	0.484459	0.496900	-7.807004
HCO	-22.288737	0.430677	0.444700	-8.799560
HCl	-15.627044	0.164814	0.171000	-3.881629
HF	-24.938080	0.209552	0.226100	-10.384114
HOCl	-31.632890	0.247073	0.264700	-11.061366
Li2	-0.432372	0.031075	0.038900	-4.910377
LiF	-24.639077	0.211447	0.222000	-6.622126
LiH	-0.795699	0.093504	0.092430	0.673966
N2	-19.954026	0.351129	0.364600	-8.453201
N2H4	-22.286544	0.677462	0.699600	-13.891975
NH	-10.440530	0.137535	0.133500	2.531993

2.7.3 $\mu = 0$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.996113				5
C	-5.415582				7
Cl	-14.941294				15
F	-24.190210				6
H	-0.498770				1
Li	-0.200729				1
N	-9.783480				6
Na	-0.187500				1
O	-15.894959				9
P	-6.462693				6
S	-10.109762				19
Si	-3.762672				9
BeH	-1.583115	0.088232	0.079400	5.541972	12
C2H2	-12.488328	0.659624	0.642400	10.808245	47
C2H4	-13.736638	0.910393	0.899000	7.149120	95
C2H6	-14.966045	1.142260	1.136900	3.363185	95
CH	-6.048946	0.134595	0.133900	0.435808	18
$CH2_{1A1}$	-6.698453	0.285331	0.288900	-2.239894	23
$CH2_{3B1}$	-6.721641	0.308519	0.304100	2.772746	17
CH3	-7.405463	0.493570	0.490800	1.738166	17
CH3Cl	-22.490905	0.637718	0.631000	4.215912	191
CH4	-8.080312	0.669649	0.670300	-0.408667	23
CN	-15.507119	0.308057	0.288800	12.084231	119
CO	-21.735532	0.424992	0.413700	7.085892	47
CO2	-37.861631	0.656132	0.621400	21.794739	95
CS	-15.811131	0.285787	0.274000	7.396201	47
Cl2	-29.991930	0.109342	0.094000	9.627435	47
ClF	-39.247872	0.116368	0.100100	10.208333	95
ClO	-30.963320	0.127067	0.104700	14.035822	154
F2	-48.459420	0.079000	0.062200	10.541862	11
H2CO	-22.919626	0.611545	0.596700	9.315159	95
H2O	-17.255335	0.362836	0.371900	-5.687902	11
H2O2	-33.220095	0.432637	0.429400	2.031210	95
H2S	-11.398296	0.290993	0.292000	-0.631958	47
H3COH	-24.128034	0.822412	0.818700	2.329429	383
H3CSH	-18.281264	0.760838	0.757000	2.408673	383
HCN	-16.213189	0.515356	0.496900	11.581428	47
HCO	-22.271978	0.462668	0.444700	11.275066	107
HCl	-15.610265	0.170201	0.171000	-0.501417	23
HF	-24.906845	0.217864	0.226100	-5.168297	5
HOCl	-31.609821	0.274799	0.264700	6.336979	191
Li2	-0.428651	0.027192	0.038900	-7.346835	5
LiF	-24.608638	0.217698	0.222000	-2.699415	23
LiH	-0.783831	0.084331	0.092430	-5.081944	5
N2	-19.947110	0.380149	0.364600	9.757363	11
N2H4	-22.265074	0.703032	0.699600	2.153374	191
NH	-10.420125	0.137874	0.133500	2.744896	9

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		Nd
Be	-0.998257	0.000053	0.000000	0.000075				
C	-5.416982	0.000100	0.000000	0.000142				
Cl	-14.941523	0.000161	0.000000	0.000228				1
F	-24.189470	0.000252	0.000000	0.000356				
H	-0.500003	0.000003	0.000000	0.000004				
Li	-0.196353	0.000001	0.000000	0.000001				
N	-9.789185	0.000093	0.000000	0.000132				
Na	-0.182093	0.000011	0.000000	0.000016				
O	-15.893033	0.000140	0.000000	0.000197				
P	-6.462550	0.000105	0.000000	0.000148				
S	-10.108931	0.000147	0.000000	0.000208				1
Si	-3.758660	0.000096	0.000000	0.000135				
BeH	-1.588246	0.000084	0.089987	0.000099	0.079400	6.643330	0.062381	1
C2H2	-12.491964	0.000440	0.657994	0.000483	0.642400	9.785361	0.303235	4
C2H4	-13.744427	0.000251	0.910452	0.000322	0.899000	7.186096	0.202087	9
C2H6	-14.986022	0.000351	1.152040	0.000405	1.136900	9.500747	0.253828	9
CH	-6.050004	0.000152	0.133019	0.000182	0.133900	-0.552744	0.114077	1
$CH2_{1A1}$	-6.705378	0.000195	0.288390	0.000219	0.288900	-0.319736	0.137646	2
$CH2_{3B1}$	-6.726726	0.000187	0.309738	0.000212	0.304100	3.538175	0.133286	1
CH3	-7.414007	0.000222	0.497017	0.000244	0.490800	3.901101	0.152954	1
CH3Cl	-22.495070	0.000373	0.636557	0.000419	0.631000	3.486858	0.262726	19
CH4	-8.094375	0.000303	0.677381	0.000319	0.670300	4.443631	0.200209	2
CN	-15.490216	0.000461	0.284049	0.000481	0.288800	-2.981091	0.302079	11
CO	-21.725909	0.000482	0.415893	0.000512	0.413700	1.376401	0.321142	4
CO2	-37.831330	0.000385	0.628281	0.000486	0.621400	4.317775	0.305191	9
CS	-15.797010	0.000397	0.271097	0.000435	0.274000	-1.821748	0.272866	4
Cl2	-29.976935	0.000242	0.093889	0.000403	0.094000	-0.069604	0.253162	4
ClF	-39.228659	0.000390	0.097667	0.000492	0.100100	-1.527010	0.308621	9
ClO	-30.934421	0.000293	0.099865	0.000362	0.104700	-3.034285	0.227314	15
F2	-48.429157	0.000362	0.050217	0.000621	0.062200	-7.519357	0.389442	1
H2CO	-22.910746	0.000299	0.600725	0.000345	0.596700	2.525867	0.216443	9
H2O	-17.258069	0.000281	0.365030	0.000313	0.371900	-4.310869	0.196661	1
H2O2	-33.200067	0.000342	0.413994	0.000441	0.429400	-9.667135	0.276916	9
H2S	-11.399427	0.000293	0.290491	0.000328	0.292000	-0.946842	0.205642	4
H3COH	-24.131705	0.000519	0.821679	0.000547	0.818700	1.869087	0.343160	38
H3CSH	-18.286397	0.000402	0.760473	0.000440	0.757000	2.179309	0.276279	38
HCN	-16.208257	0.000508	0.502087	0.000526	0.496900	3.254822	0.329929	4
HCO	-22.255600	0.000234	0.445582	0.000290	0.444700	0.553312	0.182042	10
HCl	-15.612188	0.000262	0.170662	0.000308	0.171000	-0.211815	0.193041	2
HF	-24.909398	0.000327	0.219925	0.000412	0.226100	-3.874563	0.258821	
HOCl	-31.593907	0.000403	0.259348	0.000456	0.264700	-3.358706	0.286314	19
Li2	-0.427836	0.000061	0.035130	0.000061	0.038900	-2.366012	0.038336	
LiF	-24.609450	0.000421	0.223627	0.000491	0.222000	1.021071	0.308070	2
LiH	-0.788011	0.000060	0.091655	0.000060	0.092430	-0.486213	0.037934	
N2	-19.935320	0.000390	0.356951	0.000433	0.364600	-4.799910	0.271597	1
N2H4	-22.263537	0.000345	0.685156	0.000393	0.699600	-9.063858	0.246605	19
NH	-10.419103	0.000148	0.129915	0.000175	0.133500	-2.249665	0.110000	

2.7.4 $\mu = 1/4$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.995133				42
C	-5.418574				5
Cl	-14.940577				124
F	-24.192413				8
H	-0.500154				1
Li	-0.199046				1
N	-9.788884				5
Na	-0.184711				1
O	-15.896924				6
P	-6.462873				91
S	-10.109115				144
Si	-3.760778				65
BeH	-1.585287	0.089999	0.079400	6.651146	19
C2H2	-12.490143	0.652687	0.642400	6.454958	569
C2H4	-13.739967	0.902201	0.899000	2.008897	2140
C2H6	-14.973563	1.135490	1.136900	-0.885053	5884
CH	-6.050076	0.131348	0.133900	-1.601662	59
$CH2_{1A1}$	-6.699553	0.280670	0.288900	-5.164125	120
$CH2_{3B1}$	-6.724838	0.305955	0.304100	1.164258	79
CH3	-7.408267	0.489230	0.490800	-0.985183	328
CH3Cl	-22.491578	0.631964	0.631000	0.605081	10875
CH4	-8.083269	0.664078	0.670300	-3.904097	515
CN	-15.503126	0.295668	0.288800	4.309557	721
CO	-21.740138	0.424640	0.413700	6.864805	340
CO2	-37.865186	0.652764	0.621400	19.680965	1846
CS	-15.805438	0.277750	0.274000	2.352969	1350
Cl2	-29.986173	0.105019	0.094000	6.914315	1326
ClF	-39.248441	0.115450	0.100100	9.632539	829
ClO	-30.960447	0.122946	0.104700	11.449436	1504
F2	-48.462443	0.077616	0.062200	9.673703	26
H2CO	-22.923565	0.607758	0.596700	6.939081	1382
H2O	-17.259107	0.361874	0.371900	-6.291285	23
H2O2	-33.225897	0.431740	0.429400	1.468151	2870
H2S	-11.395256	0.285833	0.292000	-3.869862	345
H3COH	-24.135671	0.819556	0.818700	0.537234	12607
H3CSH	-18.282185	0.753880	0.757000	-1.957882	38269
HCN	-16.215047	0.507435	0.496900	6.610525	781
HCO	-22.275088	0.459436	0.444700	9.246837	1986
HCl	-15.608648	0.167917	0.171000	-1.934630	290
HF	-24.910577	0.218040	0.226100	-5.076654	5
HOCl	-31.610886	0.273230	0.264700	5.352862	8312
Li2	-0.427563	0.029470	0.038900	-5.917275	25
LiF	-24.614436	0.222976	0.222000	0.612559	23
LiH	-0.785150	0.085949	0.092430	-4.066948	1
N2	-19.950249	0.372482	0.364600	4.946099	200
N2H4	-22.272004	0.693620	0.699600	-3.752678	13079
NH	-10.421403	0.132365	0.133500	-0.712094	16

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		No
Be	-1.002938	0.000039	0.000000	0.000055				
C	-5.417876	0.000075	0.000000	0.000106				
Cl	-14.944556	0.000140	0.000000	0.000199				1
F	-24.189626	0.000167	0.000000	0.000237				
H	-0.500003	0.000003	0.000000	0.000004				
Li	-0.196353	0.000001	0.000000	0.000001				
N	-9.789256	0.000069	0.000000	0.000098				
Na	-0.182093	0.000011	0.000000	0.000016				
O	-15.892887	0.000052	0.000000	0.000074				
P	-6.464934	0.000111	0.000000	0.000157				
S	-10.112105	0.000039	0.000000	0.000056				1
Si	-3.760396	0.000027	0.000000	0.000039				
BeH	-1.589059	0.000072	0.086118	0.000082	0.079400	4.215448	0.051571	
C2H2	-12.494091	0.000117	0.658333	0.000190	0.642400	9.997862	0.119078	5
C2H4	-13.746601	0.000181	0.910837	0.000235	0.899000	7.427667	0.147410	21
C2H6	-14.986311	0.000323	1.150541	0.000356	1.136900	8.559772	0.223334	58
CH	-6.051364	0.000138	0.133485	0.000157	0.133900	-0.260635	0.098622	
$CH2_{1A1}$	-6.707476	0.000171	0.289594	0.000187	0.288900	0.435632	0.117236	1
$CH2_{3B1}$	-6.727407	0.000155	0.309525	0.000172	0.304100	3.404335	0.108012	
CH3	-7.414577	0.000228	0.496692	0.000240	0.490800	3.697052	0.150812	3
CH3Cl	-22.499493	0.000431	0.637051	0.000459	0.631000	3.797375	0.288136	108
CH4	-8.095278	0.000370	0.677390	0.000377	0.670300	4.449199	0.236721	5
CN	-15.495774	0.000580	0.288642	0.000588	0.288800	-0.099272	0.369232	7
CO	-21.728158	0.000517	0.417395	0.000525	0.413700	2.318495	0.329371	3
CO2	-37.832935	0.000818	0.629285	0.000828	0.621400	4.947609	0.519360	18
CS	-15.804483	0.000424	0.274501	0.000433	0.274000	0.314488	0.271590	13
Cl2	-29.984598	0.000373	0.095485	0.000467	0.094000	0.932063	0.292734	13
ClF	-39.231612	0.000339	0.097430	0.000403	0.100100	-1.675158	0.253047	8
ClO	-30.939375	0.000253	0.101932	0.000294	0.104700	-1.736998	0.184625	15
F2	-48.430097	0.000224	0.050846	0.000403	0.062200	-7.125030	0.252866	
H2CO	-22.913163	0.000281	0.602393	0.000296	0.596700	3.572645	0.185497	13
H2O	-17.257894	0.000247	0.365002	0.000253	0.371900	-4.328755	0.158499	
H2O2	-33.202749	0.000358	0.416969	0.000373	0.429400	-7.800661	0.233981	28
H2S	-11.402570	0.000078	0.290459	0.000088	0.292000	-0.967113	0.055028	3
H3COH	-24.133042	0.000486	0.822267	0.000495	0.818700	2.238148	0.310451	126
H3CSH	-18.290270	0.000611	0.760277	0.000617	0.757000	2.056450	0.387332	382
HCN	-16.210974	0.000560	0.503839	0.000569	0.496900	4.354451	0.356994	7
HCO	-22.257793	0.000227	0.447026	0.000244	0.444700	1.459740	0.153371	19
HCl	-15.615072	0.000064	0.170513	0.000154	0.171000	-0.305878	0.096843	2
HF	-24.908978	0.000225	0.219349	0.000280	0.226100	-4.236047	0.175771	
HOCl	-31.597675	0.000535	0.260229	0.000556	0.264700	-2.805717	0.348806	83
Li2	-0.430271	0.000068	0.037564	0.000068	0.038900	-0.838362	0.042777	
LiF	-24.609492	0.000101	0.223513	0.000195	0.222000	0.949174	0.122562	
LiH	-0.788002	0.000039	0.091645	0.000039	0.092430	-0.492316	0.024461	
N2	-19.938355	0.000398	0.359843	0.000421	0.364600	-2.985240	0.264476	2
N2H4	-22.265279	0.000350	0.686756	0.000377	0.699600	-8.059900	0.236267	130
NH	-10.419028	0.000123	0.129769	0.000141	0.133500	-2.341308	0.088359	

2.7.5 $\mu = 1/2$

1. CIPSI

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol	Ndet
Be	-0.999244				53
C	-5.426998				292
Cl	-14.947964				3297
F	-24.217393				222
H	-0.503289				1
Li	-0.196938				1
N	-9.803449				161
Na	-0.182546				1
O	-15.916012				314
P	-6.465937				1155
S	-10.113623				2548
Si	-3.760405				1064
BeH	-1.588237	0.085704	0.079400	3.955757	832
C2H2	-12.494691	0.634115	0.642400	-5.198991	44849
C2H4	-13.748208	0.881053	0.899000	-11.261902	176223
C2H6	-14.988175	1.114441	1.136900	-14.093331	1730917
CH	-6.056113	0.125825	0.133900	-5.067187	1347
$CH2_{1A1}$	-6.706420	0.272842	0.288900	-10.076400	6122
$CH2_{3B1}$	-6.733935	0.300358	0.304100	-2.348100	7896
CH3	-7.417628	0.480761	0.490800	-6.299356	22475
CH3Cl	-22.501861	0.617031	0.631000	-8.765633	1481325
CH4	-8.093577	0.653421	0.670300	-10.591717	152351
CN	-15.503961	0.273514	0.288800	-9.592282	48132
CO	-21.750950	0.407940	0.413700	-3.614443	28515
CO2	-37.881120	0.622099	0.621400	0.438449	205259
CS	-15.804719	0.264098	0.274000	-6.213870	210314
Cl2	-29.991909	0.095982	0.094000	1.243454	744248
ClF	-39.267335	0.101978	0.100100	1.178535	91236
ClO	-30.969026	0.105051	0.104700	0.220009	218230
F2	-48.491509	0.056722	0.062200	-3.437436	12994
H2CO	-22.936125	0.586536	0.596700	-6.378001	96920
H2O	-17.275666	0.353076	0.371900	-11.812535	6385
H2O2	-33.245714	0.407112	0.429400	-13.985917	224948
H2S	-11.399974	0.279772	0.292000	-7.673428	24580
H3COH	-24.155854	0.799686	0.818700	-11.931540	767277
H3CSH	-18.290088	0.736309	0.757000	-12.983950	1471543
HCN	-16.220032	0.486295	0.496900	-6.654462	90087
HCO	-22.285095	0.438795	0.444700	-3.705432	264646
HCl	-15.615378	0.164125	0.171000	-4.314148	11828
HF	-24.934444	0.213761	0.226100	-7.742622	2438
HOCl	-31.623491	0.256226	0.264700	-5.317269	833425
Li2	-0.429619	0.035744	0.038900	-1.980329	180
LiF	-24.637272	0.222941	0.222000	0.590569	43868
LiH	-0.786895	0.086668	0.092430	-3.615549	395
N2	-19.957050	0.350153	0.364600	-9.065931	13243
N2H4	-22.287467	0.667412	0.699600	-20.198424	852894
NH	-10.433384	0.126646	0.133500	-4.300974	4446

2. DMC

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol		
Be	-1.008936	0.000023	0.000000	0.000033				
C	-5.423260	0.000076	0.000000	0.000107				
Cl	-14.954148	0.000202	0.000000	0.000286				
F	-24.191477	0.000252	0.000000	0.000356				
H	-0.500003	0.000003	0.000000	0.000004				
Li	-0.196353	0.000001	0.000000	0.000001				
N	-9.791893	0.000090	0.000000	0.000127				
Na	-0.182093	0.000011	0.000000	0.000016				
O	-15.894937	0.000166	0.000000	0.000235				
P	-6.470693	0.000131	0.000000	0.000185				
S	-10.120612	0.000159	0.000000	0.000225				
Si	-3.764505	0.000087	0.000000	0.000123				
BeH	-1.591076	0.000014	0.082138	0.000027	0.079400	1.717998	0.017147	
C2H2	-12.498281	0.000132	0.651757	0.000201	0.642400	5.871354	0.126046	4
C2H4	-13.750918	0.000161	0.904388	0.000221	0.899000	3.380793	0.138658	17
C2H6	-14.988213	0.000510	1.141676	0.000532	1.136900	2.997250	0.333909	173
CH	-6.057662	0.000209	0.134400	0.000222	0.133900	0.313648	0.139280	
$CH2_{1A1}$	-6.713371	0.000052	0.290105	0.000092	0.288900	0.756312	0.057541	
$CH2_{3B1}$	-6.729564	0.000048	0.306299	0.000090	0.304100	1.379802	0.056494	
CH3	-7.416224	0.000080	0.492956	0.000111	0.490800	1.352668	0.069349	2
CH3Cl	-22.507086	0.000639	0.629669	0.000675	0.631000	-0.835019	0.423506	148
CH4	-8.094495	0.000511	0.671224	0.000517	0.670300	0.579631	0.324427	15
CN	-15.503381	0.001043	0.288228	0.001049	0.288800	-0.358890	0.658412	4
CO	-21.735123	0.000184	0.416926	0.000259	0.413700	2.024133	0.162516	2
CO2	-37.840680	0.000532	0.627546	0.000632	0.621400	3.856748	0.396313	20
CS	-15.817930	0.000160	0.274059	0.000238	0.274000	0.036753	0.149415	21
Cl2	-30.003285	0.000697	0.094989	0.000806	0.094000	0.620667	0.505577	74
ClF	-39.242135	0.000505	0.096510	0.000599	0.100100	-2.252912	0.376015	9
ClO	-30.951000	0.000517	0.101915	0.000580	0.104700	-1.747928	0.363737	21
F2	-48.435978	0.000535	0.053024	0.000735	0.062200	-5.758056	0.461165	1
H2CO	-22.917290	0.000421	0.599087	0.000459	0.596700	1.497898	0.288045	9
H2O	-17.259667	0.000126	0.364724	0.000209	0.371900	-4.502851	0.130863	
H2O2	-33.208496	0.001298	0.418616	0.001339	0.429400	-6.767230	0.840434	22
H2S	-11.410768	0.000106	0.290151	0.000191	0.292000	-1.160352	0.120076	2
H3COH	-24.140019	0.000912	0.821810	0.000930	0.818700	1.951836	0.583651	76
H3CSH	-18.294070	0.000783	0.750187	0.000803	0.757000	-4.274967	0.503869	147
HCN	-16.212033	0.001145	0.496877	0.001151	0.496900	-0.014286	0.722279	9
HCO	-22.263218	0.000376	0.445018	0.000418	0.444700	0.199498	0.262080	26
HCl	-15.624439	0.000606	0.170288	0.000639	0.171000	-0.446721	0.400937	1
HF	-24.913752	0.001045	0.222272	0.001075	0.226100	-2.402033	0.674472	
HOCl	-31.609230	0.000708	0.260142	0.000755	0.264700	-2.860417	0.473654	83
Li2	-0.431518	0.000011	0.038811	0.000011	0.038900	-0.055827	0.006934	
LiF	-24.610026	0.000241	0.222196	0.000349	0.222000	0.122718	0.218790	4
LiH	-0.788462	0.000043	0.092105	0.000043	0.092430	-0.203712	0.026844	
N2	-19.944826	0.000176	0.361039	0.000251	0.364600	-2.234271	0.157774	1
N2H4	-22.269712	0.000946	0.685914	0.000963	0.699600	-8.587967	0.604160	85
NH	-10.421923	0.000057	0.130027	0.000107	0.133500	-2.179318	0.066882	

2.7.6 FCI

1. CIPSI

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
	e_{cal}	ae_{cal}	ae_{nr}	ae_{diff}			
Be	-1.009626	0.000009	0.000000	0.000012			
C	-5.432164	0.000004	0.000000	0.000006			
Cl	-14.967668	0.000005	0.000000	0.000007			
F	-24.186155	0.000003	0.000000	0.000004			
H	-0.499916	0.000000		0.000000			
Li	-0.196307	0.000000		0.000000			
N	-9.798444	0.000001	0.000000	0.000002			
Na	-0.181980	0.000000		0.000000			
O	-15.897642	0.000002	0.000000	0.000003			
P	-6.476064	0.000001	0.000000	0.000002			
S	-10.128682	0.000000	0.000000	0.000001			
Si	-3.766939	0.000002	0.000000	0.000002			
BeH	-1.588951	0.000031	0.079409	0.000032	0.079400	0.005936	0.019943
C2H2	-12.499381	0.000056	0.635222	0.000057	0.642400	-4.504129	0.035633
C2H4	-13.749829	0.000755	0.885838	0.000755	0.899000	-8.259487	0.473798
C2H6	-14.976671	0.002502	1.112848	0.002502	1.136900	-15.092883	1.570321
CH	-6.064087	0.000002	0.132008	0.000005	0.133900	-1.187362	0.002922
$CH2_{1A1}$	-6.716786	0.000001	0.284791	0.000004	0.288900	-2.578570	0.002633
$CH2_{3B1}$	-6.731323	0.000002	0.299328	0.000004	0.304100	-2.994534	0.002764
CH3	-7.415727	0.000020	0.483816	0.000020	0.490800	-4.382561	0.012661
CH3Cl	-22.521516	0.001709	0.621936	0.001709	0.631000	-5.687506	1.072221
CH4	-8.093853	0.000056	0.662026	0.000056	0.670300	-5.192118	0.035136
CN	-15.513348	0.000021	0.282740	0.000022	0.288800	-3.802447	0.013682
CO	-21.738670	0.000219	0.408865	0.000219	0.413700	-3.034243	0.137599
CO2	-37.838700	0.001069	0.611253	0.001069	0.621400	-6.367363	0.670811
CS	-15.829917	0.000200	0.269071	0.000200	0.274000	-3.092953	0.125661
Cl2	-30.027659	0.000014	0.092322	0.000017	0.094000	-1.052786	0.010930
ClF	-39.249390	0.000609	0.095566	0.000609	0.100100	-2.844986	0.382114
ClO	-30.966211	0.000499	0.100901	0.000499	0.104700	-2.383929	0.313427
F2	-48.431244	0.000054	0.058933	0.000054	0.062200	-2.050000	0.033800
H2CO	-22.917424	0.000211	0.587787	0.000211	0.596700	-5.593292	0.132435
H2O	-17.256113	0.000011	0.358639	0.000011	0.371900	-8.321241	0.006951
H2O2	-33.206043	0.000566	0.410928	0.000566	0.429400	-11.591315	0.355078
H2S	-11.416822	0.000036	0.288308	0.000036	0.292000	-2.316961	0.022567
H3COH	-24.126733	0.000210	0.797264	0.000210	0.818700	-13.451386	0.131821
H3CSH	-18.303106	0.000888	0.742596	0.000888	0.757000	-9.038560	0.557191
HCN	-16.220238	0.000114	0.489715	0.000114	0.496900	-4.508747	0.071423
HCO	-22.265628	0.000503	0.435907	0.000503	0.444700	-5.517539	0.315588
HCl	-15.636332	0.000018	0.168747	0.000019	0.171000	-1.413491	0.011743
HF	-24.902433	0.000009	0.216362	0.000010	0.226100	-6.110912	0.006124
HOCl	-31.621625	0.000224	0.256399	0.000224	0.264700	-5.208797	0.140532
Li2	-0.431443	0.000004	0.038829	0.000004	0.038900	-0.044823	0.002472
LiF	-24.599582	0.000001	0.217120	0.000003	0.222000	-3.062355	0.001982
LiH	-0.787778	0.000003	0.091555	0.000003	0.092430	-0.549078	0.002108
N2	-19.952215	0.000053	0.355328	0.000053	0.364600	-5.818524	0.033494

2.8 Python code to export Data in csv format

```
for basis in ['dz', 'tz', 'qz']:
   for method in ['ccsdt','pbe','pbe0','blyp','b3lyp']:
      name = basis+'-'+method
      print(":var "+name.replace('-','_').replace('.','')+"="+name)

   for method in ['cipsi', 'dmc']:
     for mu in ['0.00', '0.25', '0.50']:
name = basis+'-'+method+'-'+mu
print(":var "+name.replace('-','_').replace('.','')+"="+name)
   if basis == 'dz':
     for method in ['cipsi', 'dmc']:
for mu in ['1.00', '2.00', '5.00', 'inf']:
   name = basis+'-'+method+'-'+mu
   print(":var "+name.replace('-','_').replace('.','')+"="+name)
   elif basis == 'tz':
     for method in ['cipsi', 'dmc']:
       for mu in ['1.00']:
  name = basis+'-'+method+'-'+mu
  print(":var "+name.replace('-','_').replace('.','')+"="+name)


print("Basis,Method,Mu,Molecule,TotalEnergy,TotalEnergyErr,AtomizationEnergy,Atomizati

def print_data(x,basis,method,mu):
  ndet = ","
  if mu is None:
    mu = ""
  if len(x[0]) == 5:
    for line in x[2:]:
      if line[0] != "":
if mu == "opt":
  ndet = ""
elif mu is not "":
  ndet = line[-1]
  line = [ line[0], line[1], "", line[2], ""]
  line = ",".join([str(x) for x in line[:5]])
  print (f"{basis},{method},{mu},{line},{ndet}")
  else:
    for line in x[2:]:
```

```
      if line[0] != "":
if mu == "opt":
  ndet = ""
elif mu is not "":
  ndet = line[-1]
  line = ",".join([str(x) for x in line[:5]])
  print (f"{basis},{method},{mu},{line},{ndet}")

data = [ (dz_ccsdt,"VDZ-BFD","CCSD(T)",None),
 (dz_pbe,"VDZ-BFD","PBE",None),
 (dz_pbe0,"VDZ-BFD","PBE0",None),
 (dz_blyp,"VDZ-BFD","BLYP",None),
 (dz_b3lyp,"VDZ-BFD","B3LYP",None),
 (dz_cipsi_000,"VDZ-BFD","CIPSI","0.00"),
 (dz_cipsi_025,"VDZ-BFD","CIPSI","0.25"),
 (dz_cipsi_050,"VDZ-BFD","CIPSI","0.50"),
 (dz_cipsi_100,"VDZ-BFD","CIPSI","1.00"),
 (dz_cipsi_200,"VDZ-BFD","CIPSI","2.00"),
 (dz_cipsi_500,"VDZ-BFD","CIPSI","5.00"),
 (dz_cipsi_inf,"VDZ-BFD","CIPSI","inf"),
 (tz_cipsi_inf,"VTZ-BFD","CIPSI","inf"),
 (qz_cipsi_inf,"VQZ-BFD","CIPSI","inf"),
 (dz_dmc_000,"VDZ-BFD","DMC","0.00"),
 (dz_dmc_025,"VDZ-BFD","DMC","0.25"),
 (dz_dmc_050,"VDZ-BFD","DMC","0.50"),
 (dz_dmc_100,"VDZ-BFD","DMC","1.00"),
 (dz_dmc_200,"VDZ-BFD","DMC","2.00"),
 (dz_dmc_500,"VDZ-BFD","DMC","5.00"),
 (dz_dmc_inf,"VDZ-BFD","DMC","inf"),
 (dz_dmc_opt,"VDZ-BFD","DMC","opt"),
 (tz_ccsdt,"VTZ-BFD","CCSD(T)",None),
 (tz_pbe,"VTZ-BFD","PBE",None),
 (tz_pbe0,"VTZ-BFD","PBE0",None),
 (tz_blyp,"VTZ-BFD","BLYP",None),
 (tz_b3lyp,"VTZ-BFD","B3LYP",None),
 (tz_cipsi_000,"VTZ-BFD","CIPSI","0.00"),
 (tz_cipsi_025,"VTZ-BFD","CIPSI","0.25"),
 (tz_cipsi_050,"VTZ-BFD","CIPSI","0.50"),
 (tz_dmc_000,"VTZ-BFD","DMC","0.00"),
 (tz_dmc_025,"VTZ-BFD","DMC","0.25"),
```

```
 (tz_dmc_050,"VTZ-BFD","DMC","0.50"),
 (tz_cipsi_100,"VTZ-BFD","CIPSI","1.00"),
 (tz_dmc_100,"VTZ-BFD","DMC","1.00"),
 (qz_ccsdt,"VQZ-BFD","CCSD(T)",None),
 (qz_pbe,"VQZ-BFD","PBE",None),
 (qz_pbe0,"VQZ-BFD","PBE0",None),
 (qz_blyp,"VQZ-BFD","BLYP",None),
 (qz_b3lyp,"VQZ-BFD","B3LYP",None),
 (qz_cipsi_000,"VQZ-BFD","CIPSI","0.00"),
 (qz_cipsi_025,"VQZ-BFD","CIPSI","0.25"),
 (qz_cipsi_050,"VQZ-BFD","CIPSI","0.50"),
 (qz_dmc_000,"VQZ-BFD","DMC","0.00"),
 (qz_dmc_025,"VQZ-BFD","DMC","0.25"),
 (qz_dmc_050,"VQZ-BFD","DMC","0.50"),
]

# Extract reference data from a random data table
ref = [ [ x[0], " ", " ", x[5] ] for x in qz_dmc_000 if x[5] != ""]
print_data(ref, "", "Reference", "")

for name, basis, method, mu in data:
  print_data(name, basis, method, mu)

rsdft.csv
```

3 Data for plots

3.1 Initialize R packages

```
to_kcal <- 627.502164882
library(ggplot2)
library(latex2exp)
library(extrafont)
library(RColorBrewer)
loadfonts()
```

3.2 Read csv

```
mad = function(x) { mean(abs(x)) }
raw_data <- read.csv("rsdft.csv")
```

```
ref <- subset(raw_data, Method == "Reference")[c("Molecule","AtomizationEnergy")]

tmp <- subset(raw_data, (Method == "DMC" & Basis == "VTZ-BFD" & AtomizationEnergy != 0

get_ref = function(name) {
    l <- subset(ref,(Molecule == name))$"AtomizationEnergy"
    ifelse( length(l) == 0, 0.,l[1])
}
raw_data$ref <- sapply(raw_data$"Molecule", get_ref)
raw_data$ae.diff <- (raw_data$"AtomizationEnergy" - raw_data$ref) * to_kcal
summary(raw_data)
```

```
   Error in read.table(file = file, header = header, sep = sep, quote = quote,  :
     more columns than column names
```

```
Basis          Method           Mu          Molecule     TotalEnergy
   :  55   CIPSI  :1071          :1060   BeH    :  47   Min.   :-48.5039
    VDZ-BFD:1340   DMC    :1005   0.00   : 402   C2H2   :  47   1st Qu.:-22.4809
    VQZ-BFD: 804   B3LYP  : 201   0.25   : 402   C2H4   :  47   Median :-14.9413
    VTZ-BFD: 937   BLYP   : 201   0.50   : 402   C2H6   :  47   Mean   :-15.5174
   CCSD(T): 201   1.00   : 268   CH     :  47   3rd Qu.: -6.7063
   PBE    : 201   inf    : 267   CH2_1A1:  47   Max.   : -0.1742
   (Other): 256   (Other): 335   (Other):2854   NA's   :55
    TotalEnergyErr   AtomizationEnergy AtomizationEnergyErr      Ndet
    Min.   :0.0000   Min.   :0.0000    Min.   :-75.1781     Min.   :       0
    1st Qu.:0.0002   1st Qu.:0.1387    1st Qu.: -2.3366     1st Qu.:      23
    Median :0.0007   Median :0.2681    Median :  0.0002     Median :     394
    Mean   :0.1276   Mean   :0.3251    Mean   : -2.7038     Mean   : 1176081
    3rd Qu.:0.2046   3rd Qu.:0.4619    3rd Qu.:  0.0006     3rd Qu.:   41778
    Max.   :1.1423   Max.   :1.1520    Max.   : 21.7947     Max.   :19555662
    NA's   :1216     NA's   :381       NA's   :1252         NA's   :1165
 ref             ae.diff
    Min.   :0.00000   Min.   :-70.6994
    1st Qu.:0.09243   1st Qu.: -5.9057
    Median :0.24300   Median : -0.3853
    Mean   :0.29081   Mean   : -3.7199
    3rd Qu.:0.42940   3rd Qu.:  0.0000
    Max.   :1.13690   Max.   : 12.6322
```

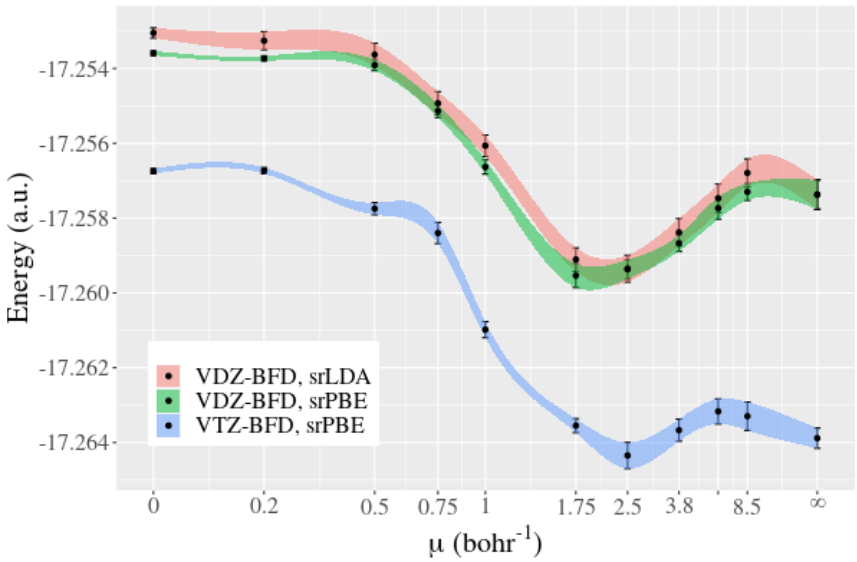
```
      NA's   :381
```

3.3 Figure 2 (H_2O)

μ		N_{det}	E(DMC,srPBE,DZ)	Error	N_{det}	E(DMC,srPBE,TZ)
0.00	0.0000000000	11	-17.2535927658	0.0000616883	23	-17.2567442368
0.20	0.1666666700	23	-17.2537299553	0.0000673868	23	-17.2567293499
0.50	0.3333333300	1442	-17.2539120512	0.0001475010	1699	-17.2577489156
0.75	0.4285714300	3213	-17.2551351593	0.0001757492	13362	-17.2583975528
1.00	0.5000000000	6743	-17.2566320269	0.0001881680	25673	-17.2609826285
1.75	0.6363636400	54540	-17.2595366309	0.0003193539	207475	-17.2635480054
2.50	0.7142857100	51691	-17.2593693798	0.0002564347	858123	-17.2643468817
3.80	0.7916666700	103059	-17.2586706893	0.0002222800	1621513	-17.2636697373
5.70	0.8507462700	102599	-17.2577349871	0.0002927319	1629655	-17.2631675892
8.50	0.8947368400	101803	-17.2572986405	0.0002283964	1643301	-17.2632963114
inf	1.0000000000	255971	-17.257373	0.0003928008	1631982	-17.2638832283

```
vdz        = data["X"]
vdz$"E"    = data$"E.DMC.srPBE.DZ."
vdz$"E.lo" = data$"E.DMC.srPBE.DZ." - data$"Error"
vdz$"E.hi" = data$"E.DMC.srPBE.DZ." + data$"Error"
vdz$Basis  = "VDZ-BFD, srPBE"
vdz.spline_int <- as.data.frame(spline(vdz$X, vdz$E, n=101, method="natural"))
vdz.spline_int$"E.hi" <- as.data.frame(spline(vdz$X, vdz$E.hi, n=101, method="natural"
vdz.spline_int$"E.lo" <- as.data.frame(spline(vdz$X, vdz$E.lo, n=101, method="natural"
vdz.spline_int$X <- vdz.spline_int$x
vdz.spline_int$E <- vdz.spline_int$y
vdz.spline_int$Basis <- "VDZ-BFD, srPBE"

vtz        = data["X"]
vtz$"E"    = data$"E.DMC.srPBE.TZ."
vtz$"E.lo" = data$"E.DMC.srPBE.TZ." - data$"Error.1"
vtz$"E.hi" = data$"E.DMC.srPBE.TZ." + data$"Error.1"
vtz$Basis  = "VTZ-BFD, srPBE"
vtz.spline_int <- as.data.frame(spline(vtz$X, vtz$E, n=101, method="natural"))
vtz.spline_int$"E.hi" <- as.data.frame(spline(vtz$X, vtz$E.hi, n=101, method="natural"
vtz.spline_int$"E.lo" <- as.data.frame(spline(vtz$X, vtz$E.lo, n=101, method="natural"
vtz.spline_int$X <- vtz.spline_int$x
vtz.spline_int$E <- vtz.spline_int$y
vtz.spline_int$Basis <- "VTZ-BFD, srPBE"
```

```
lda        = data["X"]
lda$"E"    = data$"E.DMC.srLDA.DZ."
lda$"E.lo" = data$"E.DMC.srLDA.DZ." - data$"Error.2"
lda$"E.hi" = data$"E.DMC.srLDA.DZ." + data$"Error.2"
lda$Basis  = "VDZ-BFD, srLDA"
lda.spline_int <- as.data.frame(spline(lda$X, lda$E, n=101, method="natural"))
lda.spline_int$E.hi <- as.data.frame(spline(lda$X, lda$E.hi, n=101, method="natural"))$
lda.spline_int$E.lo <- as.data.frame(spline(lda$X, lda$E.lo, n=101, method="natural"))$
lda.spline_int$X <- lda.spline_int$x
lda.spline_int$E <- lda.spline_int$y
lda.spline_int$Basis <- "VDZ-BFD, srLDA"

d = rbind(lda,vdz,vtz)
ds = rbind(lda.spline_int,vdz.spline_int,vtz.spline_int)

breaks <- data$"X"
labels <- data$"X..mu"
labels[9] <- ""
labels[11] <- TeX("$\\infty$")

p <- ggplot(ds, aes(x=X, y=E, ymin=E.lo, ymax=E.hi, fill=Basis ))
p <- p + geom_errorbar(data=d, width=0.01)
p <- p + geom_ribbon(alpha=0.5)
p <- p + geom_point(data=d)
p <- p + scale_x_continuous(name=TeX("$\\mu$ (bohr$^{-1}$)"), breaks=breaks,
                            labels=labels)
p <- p + scale_y_continuous(name = "Energy (a.u.)", breaks=seq(-17.266,-17.252,0.002))
p <- p + theme(text = element_text(size = 20, family="Times"),
               legend.position = c(.20, .20),
               legend.title = element_blank())
p
```



Export to pdf

```
pdf("../Manuscript/h2o-dmc.pdf", family="Times", width=8, height=5)
p
dev.off()
```

3.4 Comparision with Jastrow optimized wf

Parameters of the Jastrow: J_{ee} = a r_{12} / (1 + b r_{12}) J_{eN} = -(p r_{12} / (1 + p r_{12}))^2 a = 1/2 b = 0.886226925453 p_H = 0.3467 p_O = 1.1485 (energy minimization)

3.4.1 Overlap

```
normalize <- function(x) {x / sqrt(sum(x^2))}
FCI <- normalize(scan("fci.dat"))
dH2O <- data.frame(FCI)
dH2O$mu_0 <- normalize(scan("mu00.dat"))
dH2O$mu_025 <- normalize(scan("mu25.dat"))
dH2O$mu_05 <- normalize(scan("mu05.dat"))
dH2O$mu_1  <- normalize(scan("mu10.dat"))
dH2O$mu_2  <- normalize(scan("mu20.dat"))
dH2O$mu_5  <- normalize(scan("mu50.dat"))
dH2O$mu_inf<- normalize(scan("diag.dat"))
```

```
dH2O$jast  <- normalize(scan("jast.dat"))
overlap <- function(x) {x <- abs(crossprod(x,dH2O$jast)[1]) }
H2O <- apply(dH2O,2,overlap)
H2O


    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

    Read 200 items

  FCI      mu_0    mu_025     mu_05      mu_1      mu_2      mu_5    mu_inf
    0.9908628 0.9875157 0.9885532 0.9918674 0.9943390 0.9926737 0.9906157 0.9899355
 jast
    1.0000000

Mu <- c(0., 0.25, 0.5, 1., 2., 5., Inf)
X <- Mu/(Mu+1.)
X[7] <- 1.
H2O_FCI <- H2O["FCI"]
H2O <- subset(H2O, names(H2O) != "jast" & names(H2O) != "FCI")
ov = data.frame(Mu, H2O)
print(ov)
Mu <- as.character(Mu)
Mu[7] <- TeX("$\\infty$")

H2O.spline_int <- as.data.frame(spline(ov$"X", ov$"H2O", n=101))
```

```
p <- ggplot(ov, aes(x=X, y=H2O))
p <- p + geom_line(data = H2O.spline_int, aes(x=x, y=y, colour='red'),
                   show.legend=FALSE, lwd=2)
p <- p + geom_point(aes(x=X,y=H2O), lwd=2.)
p <- p + scale_x_continuous(name=TeX("$\\mu$ (bohr$^{-1}$)"), breaks=X, labels=Mu)
p <- p + scale_y_continuous(name = TeX("Overlap"))
p <- p + theme(text = element_text(size = 20, family="Times"),
               legend.position = c(.85, .15))
p
```

```
'x' and 'y' lengths differ
```

```
pdf("../Manuscript/overlap.pdf", family="Times", width=8, height=5)
p
dev.off()
```

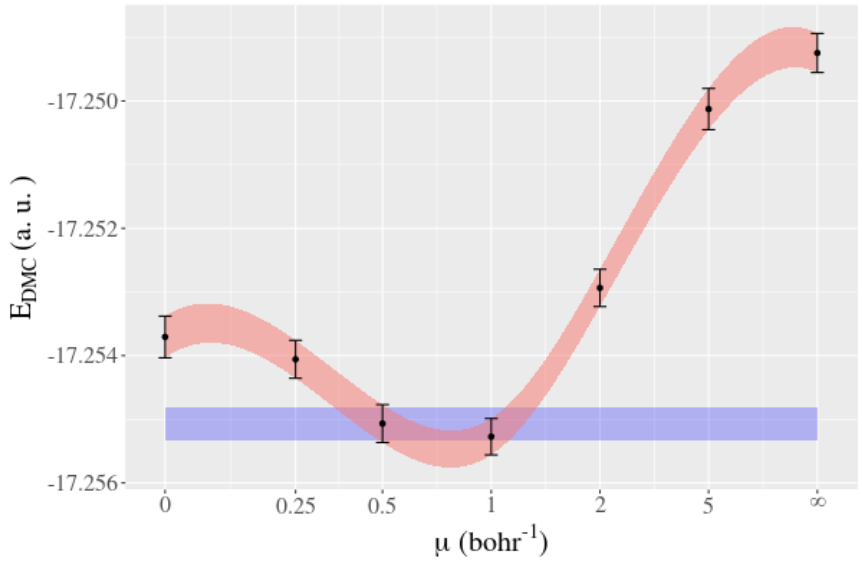
3.4.2 DMC energies

Mu	E	Error
0.00	-17.2537075442	0.0003272719
0.25	-17.2540586404	0.0002976313
0.50	-17.2550687726	0.0002976167
1.00	-17.2552742178	0.0002854467
2.00	-17.2529369035	0.0002926223
5.00	-17.2501268640	0.0003236742
Inf	-17.2492453661	0.0003067415

DMC Energy of Jastrow-optimized WF : 17.2550782462 +/- 0.0002578873

```
Mu <- c(0., 0.25, 0.5, 1., 2., 5., Inf)
data$X <- Mu/(Mu+1.)
data$X[7] <- 1.
Mu <- as.character(Mu)
Mu[7] <- TeX("$\\infty$")

Eref <- -17.2550782462
Eref_err <- 0.0002578873

x <- c(0., 1.)
Jast <- data.frame(x)
Jast$y <- c(Eref,Eref)
Jast$lo <- c(Eref-Eref_err,Eref-Eref_err)
Jast$hi <- c(Eref+Eref_err,Eref+Eref_err)
print(Jast)

E.lo <- data$E - data$Error
E.hi <- data$E + data$Error
E <- data$E
X <- data$X
H2O.spline_int <- as.data.frame(spline(X, E, n=101))
H2O.spline_int$hi <- as.data.frame(spline(X, E.hi, n=101))$y
H2O.spline_int$lo <- as.data.frame(spline(X, E.lo, n=101))$y

p <- ggplot(H2O.spline_int, aes(x=x, y=y, ymin=lo, ymax=hi, fill="red"))
p <- p + geom_ribbon(data=Jast, aes(x=x, y=y, ymin=lo, ymax=hi),
                     alpha=0.25, fill="blue", show.legend = FALSE)
p <- p + geom_ribbon(alpha=0.5, show.legend = FALSE)
```

```
p <- p + geom_point(data=data, aes(x=X, y=E, ymin=E.lo, ymax=E.hi), show.legend=FALSE)
p <- p + geom_errorbar(data=data, aes(x=X, y=E, ymin=E.lo, ymax=E.hi),
       show.legend=FALSE, width=.02)
p <- p + scale_x_continuous(name=TeX("$\\mu$ (bohr$^{-1}$)"), breaks=X, labels=Mu)
p <- p + scale_y_continuous(name = TeX("E_{DMC} (a.u.)"))
p <- p + theme(text = element_text(size = 20, family="Times") )
p
```



Export to pdf

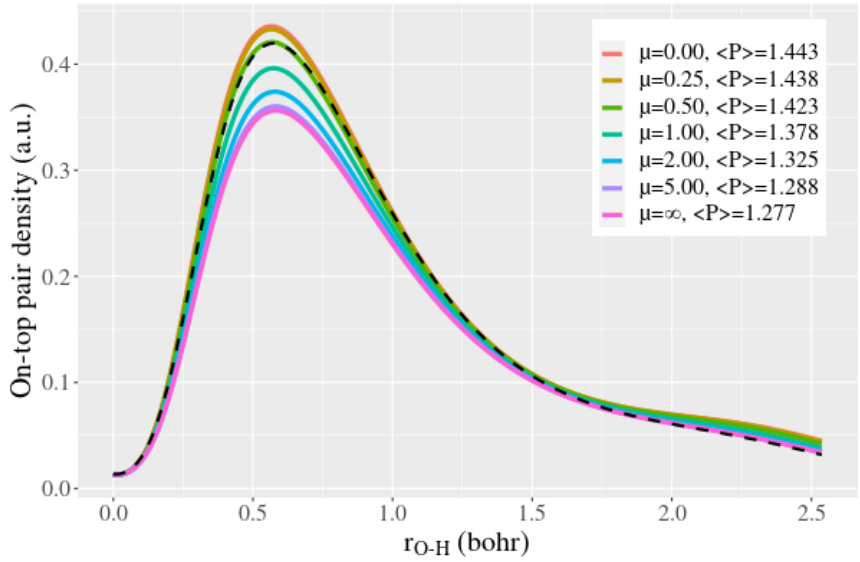
```
pdf("../Manuscript/h2o-200-dmc.pdf", family="Times", width=8, height=5)
p
dev.off()
```

3.5 On-top pair density

```
breaks <- c("0.00", "0.25", "0.50", "1.00", "2.00", "5.00", "$\\infty$", "Jastrow")

tmp_data <- read.csv("H2O_1.e-6.density")
data.0 <- data.frame(mu=breaks[1], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O_0.25.density")
data.0.25 <- data.frame(mu=breaks[2], x=tmp_data$X..distance, n=tmp_data$on.top)
```

```
tmp_data <- read.csv("H2O_0.5.density")
data.0.5 <- data.frame(mu=breaks[3], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O_1.0.density")
data.1.0 <- data.frame(mu=breaks[4], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O_2.0.density")
data.2.0 <- data.frame(mu=breaks[5], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O_5.0.density")
data.5.0 <- data.frame(mu=breaks[6], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O_1e6.density")
data.inf <- data.frame(mu=breaks[7], x=tmp_data$X..distance, n=tmp_data$on.top)

tmp_data <- read.csv("H2O.density")
data.J <- data.frame(mu=breaks[8], x=tmp_data$X..distance, n=tmp_data$on.top)


data <- rbind(data.0, data.0.25, data.0.5, data.1.0, data.2.0, data.5.0, data.inf)

labels= TeX(breaks)

labels[1] <- TeX("\u00B5=$0.00$, $<P>=1.443$")
labels[2] <- TeX("\u00B5=$0.25$, $<P>=1.438$")
labels[3] <- TeX("\u00B5=$0.50$, $<P>=1.423$")
labels[4] <- TeX("\u00B5=$1.00$, $<P>=1.378$")
labels[5] <- TeX("\u00B5=$2.00$, $<P>=1.325$")
labels[6] <- TeX("\u00B5=$5.00$, $<P>=1.288$")
labels[7] <- TeX("\u00B5=\\infty, $<P>=1.277$")
labels[8] <- TeX("Jastrow  $<P>=1.404$")

p <- ggplot(data, aes(x=x, y=n, col=mu))
p <- p + geom_line(lwd=1.5)
p <- p + geom_line(data=data.J, lwd=1, col=1, linetype="dashed")
p <- p + scale_colour_discrete(name = "", breaks = breaks,
                               labels = labels)
#p <- p + scale_color_brewer(palette = "Paired")
p <- p + scale_x_continuous(name=TeX("$r_{O-H}$ (bohr)"))
```

```
p <- p + scale_y_continuous(name = "On-top pair density (a.u.)")
p <- p + theme(text = element_text(size = 20, family="Times"),
               legend.title=element_blank(),
               legend.position=c(.81,.75), legend.text.align = 0)
p
```

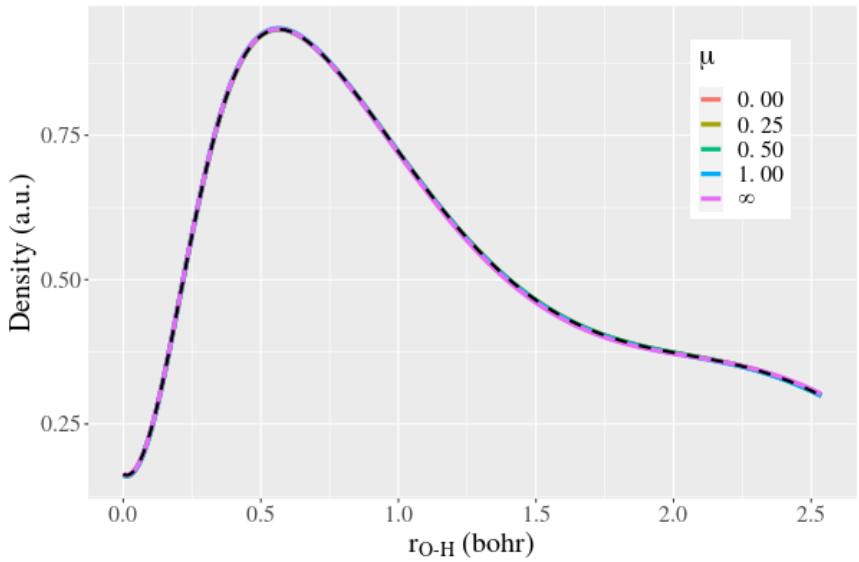



```
pdf("../Manuscript/on-top-mu.pdf", family="Times", width=8, height=5)
p
dev.off()
```

3.6 One-body density

```
breaks <- c("0.00", "0.25", "0.50", "1.00", "$\\infty$", "Jastrow")

tmp_data <- read.csv("H2O_1.e-6.density")
data.0 <- data.frame(mu=breaks[1], x=tmp_data$X..distance, n=tmp_data$density)

tmp_data <- read.csv("H2O_0.25.density")
data.0.25 <- data.frame(mu=breaks[2], x=tmp_data$X..distance, n=tmp_data$density)

tmp_data <- read.csv("H2O_0.5.density")
data.0.5 <- data.frame(mu=breaks[3], x=tmp_data$X..distance, n=tmp_data$density)
```

```
tmp_data <- read.csv("H2O_1.0.density")
data.1.0 <- data.frame(mu=breaks[4], x=tmp_data$X..distance, n=tmp_data$density)

tmp_data <- read.csv("H2O_1e6.density")
data.inf <- data.frame(mu=breaks[5], x=tmp_data$X..distance, n=tmp_data$density)

tmp_data <- read.csv("H2O.density")
data.J <- data.frame(mu=breaks[6], x=tmp_data$X..distance, n=tmp_data$density)


data <- rbind(data.0, data.0.25, data.0.5, data.1.0, data.inf)

labels= TeX(breaks)

p <- ggplot(data, aes(x=x, y=n, col=mu))
p <- p + geom_line(lwd=1.5)
p <- p + geom_line(data=data.J, lwd=1, col=1, linetype="dashed")
p <- p + scale_colour_discrete(name = TeX("$\\mu$"), breaks = breaks,
                               labels = labels)
p <- p + scale_x_continuous(name=TeX("$r_{O-H}$ (bohr)"))
p <- p + scale_y_continuous(name = "Density (a.u.)")
p <- p + theme(text = element_text(size = 20, family="Times"), legend.position=c(.85,.
p
```




```
pdf("../Manuscript/density-mu.pdf", family="Times", width=8, height=5)
p
dev.off()
```

3.7 Optimal mu

Find the optimal μ in VDZ-BFD for each molecule and atom, making a spline interpolation of the total energy wrt μ.

```
rows <- list()
j <- 0
for (mol in levels(ref$"Molecule") )
{
    data <- subset(raw_data, (Method == "DMC" & Basis == "VDZ-BFD" & Molecule == mol &
    data$"Mu" <- as.numeric(levels(factor(data$"Mu")))
    vdz        <- data["Mu"]
    vdz$"X"    <- data$"Mu"/(data$"Mu"+1.)
    vdz$"E"    <- data$"TotalEnergy"
    vdz$"E.lo" <- data$"TotalEnergy" - data$"TotalEnergyErr"
    vdz$"E.hi" <- data$"TotalEnergy" + data$"TotalEnergyErr"
    vdz$"Basis" <- "DZ"
    vdz$"X"[7] <- 1.
    vdz$"Mu"[7] <- TeX("$\\infty$")
```

```
    vdz.spline_int <- as.data.frame(spline(vdz$"X", vdz$"E", n=101))
    vdz.spline_int_lo <- as.data.frame(spline(vdz$"X", vdz$"E.lo", n=101))
    vdz.spline_int_hi <- as.data.frame(spline(vdz$"X", vdz$"E.hi", n=101))
    Emin = min(vdz.spline_int)
    i <- which(vdz.spline_int$y == Emin)
    x <- vdz.spline_int$x[i]
    Eerr <- (vdz.spline_int_hi$y - vdz.spline_int_lo$y)[i]
    mu <- x / (1-x)
    dat <- data.frame("Molecule"=mol, "Mu"=mu, "TotalEnergy"=Emin, "TotalEnergyErr"=Ee
    j <- j + 1
    rows[[j]] <- dat
}
mu_opt = do.call(rbind, rows)
mu_opt
```

	Molecule	Mu	TotalEnergy	TotalEnergyErr
1	Be	0.9607843	-1.0079614	2.173233e-05
2	BeH	0.5625000	-1.5805161	4.068057e-04
3	C	2.8461538	-5.4320135	2.059806e-04
4	C2H2	2.1250000	-12.4978013	1.693722e-03
5	C2H4	2.0303030	-13.7496647	3.523223e-03
6	C2H6	2.0303030	-14.9862617	3.724296e-03
7	CH	2.1250000	-6.0641416	4.574218e-04
8	CH2_1A1	3.3478261	-6.7168953	1.009787e-03
9	CH2_3B1	3.1666667	-6.7315432	8.764694e-04
10	CH3	1.2727273	-7.4162297	5.308939e-04
11	CH3Cl	3.5454545	-22.5123920	4.244907e-03
12	CH4	1.7777778	-8.0950234	7.120921e-04
13	Cl	Inf	-14.9623070	5.120000e-04
14	Cl2	2.5714286	-30.0152821	4.434831e-03
15	ClF	Inf	-39.2471030	2.942000e-03
16	ClO	2.7037037	-30.9557206	3.401803e-03
17	CN	2.3333333	-15.5136584	1.488025e-03
18	CO	2.4482759	-21.7422902	1.696402e-03
19	CO2	Inf	-37.8388280	3.554000e-03
20	CS	3.7619048	-15.8228209	2.003207e-03
21	F	3.1666667	-24.1949308	7.392111e-04
22	F2	4.8823529	-48.4453257	4.050066e-03

23	H	0.0000000	-0.5000310	3.600000e-05
24	H2CO	2.7037037	-22.9171504	3.310751e-03
25	H2O	2.2258065	-17.2591427	1.461277e-03
26	H2O2	13.2857143	-33.2120191	4.669681e-03
27	H2S	2.4482759	-11.4106146	3.902506e-04
28	H3COH	Inf	-24.1332880	2.934000e-03
29	H3CSH	2.4482759	-18.2993314	4.556780e-03
30	HCl	3.3478261	-15.6303711	1.893109e-03
31	HCN	2.3333333	-16.2207532	1.825870e-03
32	HCO	2.0303030	-22.2673034	3.309960e-03
33	HF	2.3333333	-24.9104641	1.191899e-03
34	HOCl	4.5555556	-31.6166964	4.824617e-03
35	Li	1.0000000	-0.1963480	2.000000e-05
36	Li2	0.7241379	-0.4314668	3.606647e-05
37	LiF	2.5714286	-24.6088294	1.550953e-03
38	LiH	2.4482759	-0.7887656	3.051500e-05
39	N	3.0000000	-9.7986423	3.119161e-04
40	N2	2.1250000	-19.9524865	1.049009e-03
41	N2H4	2.1250000	-22.2699021	4.249432e-03
42	Na	0.6129032	-0.1821443	2.783626e-05
43	Na2	0.0000000	-0.3911310	1.820000e-04
44	NaCl	1.1276596	-15.3111605	5.178434e-03
45	NH	2.3333333	-10.4264841	7.975760e-04
46	NH2	2.1250000	-11.0809890	1.361988e-03
47	NH3	1.8571429	-11.7605194	3.873311e-04
48	NO	2.3333333	-25.9345353	2.074652e-03
49	O	2.7037037	-15.9017109	5.379650e-04
50	O2	4.2631579	-31.9858780	2.794749e-03
51	OH	2.8461538	-16.5657619	1.069541e-03
52	P	2.5714286	-6.4727488	3.693117e-04
53	P2	2.8461538	-13.1215881	2.096992e-03
54	PH2	Inf	-7.7124550	8.060000e-04
55	PH3	Inf	-8.3503240	1.756000e-03
56	S	Inf	-10.1249220	3.820000e-04
57	S2	6.6923077	-20.4034041	3.266097e-03
58	Si	Inf	-3.7651370	1.260000e-04
59	Si2	4.0000000	-7.6457229	9.500469e-04
60	Si2H6	3.5454545	-11.3730815	3.866939e-03
61	SiH2_1A1	6.1428571	-5.0079099	8.651497e-04
62	SiH2_3B1	7.3333333	-4.9746405	7.553294e-04

```
   63     SiH3        Inf  -5.6243160   1.250000e-03
   64     SiH4  2.5714286  -6.2776917   9.959756e-04
   65      SiO  3.7619048 -19.9634153   1.961472e-03
   66       SO        Inf -26.2122290   4.822000e-03
   67      SO2  3.0000000 -42.2998947   6.613181e-03
```

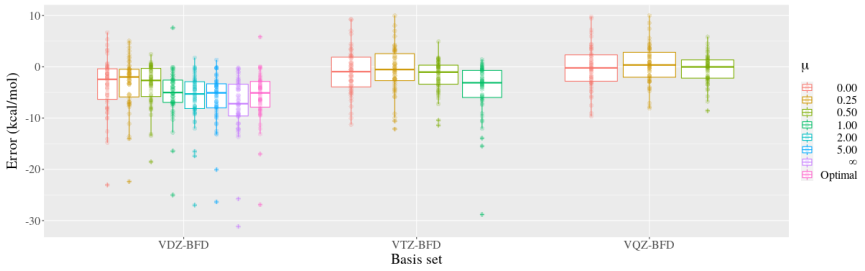
3.8 Figure MAD DZ TZ QZ

```
data <- data.frame(ref["Molecule"])
data <- subset(raw_data, (Method == "DMC" & Basis == "VDZ-BFD" & AtomizationEnergy != 0
aggregate(ae.diff~Mu, na.omit(data), mad)
```

```
    Mu  ae.diff
1 0.00 4.606710
2 0.25 4.038558
3 0.50 3.743644
4 1.00 5.417523
5 2.00 5.977186
6 5.00 6.176869
7  inf 7.631149
```

```
data <- subset(raw_data, (Method == "DMC" & AtomizationEnergy != 0.))
fill <- "#4271AE"
line <- "#1F3552"
d = data[c("Mu","ae.diff","Molecule","Basis")]
d$Mu <- factor(d$Mu)

labels <- as.character(c("0.00", "0.25", "0.50", "1.00", "2.00", "5.00", "$\\infty$")
labels[7] <- TeX(labels[7])
labels[8] <- "Optimal"
p <- ggplot(d, aes(x=Basis, y=ae.diff, color=Mu))
p <- p + scale_x_discrete(name="Basis set", limits=c("VDZ-BFD", "VTZ-BFD", "VQZ-BFD"),
                          labels=c("VDZ-BFD", "VTZ-BFD", "VQZ-BFD")
)
p <- p + scale_y_continuous(name = TeX("Error (kcal/mol)"))
p <- p + scale_colour_discrete(name = expression(mu),
                               labels = labels)
p <- p + geom_boxplot(varwidth=FALSE,alpha = 1, outlier.shape = 3)
p <- p + geom_point(position = position_dodge(.75), alpha=.2, size=3, stroke=0)
```

```
p <- p + theme(text = element_text(size = 20, family="Times"))
p
```

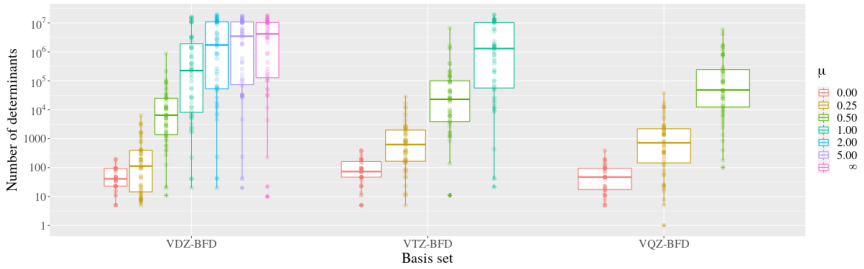



```
pdf("../Manuscript/g2-dmc.pdf", family="Times", width=16, height=5)
p
dev.off()
```

3.9 Figure Ndet DZ TZ QZ

```
data <- subset(raw_data, (Method == "DMC" & AtomizationEnergy != 0. & Mu != "opt"))
fill <- "#4271AE"
line <- "#1F3552"
d = data[c("Mu","Ndet","Molecule","Basis")]
d$Mu <- factor(d$Mu)

labels <- as.character(c("0.00", "0.25", "0.50", "1.00", "2.00", "5.00", "$\\infty$")
labels[7] <- TeX(labels[7])
labels[8] <- "Optimal"
p <- ggplot(d, aes(x=Basis, y=Ndet, color=Mu))
p <- p + scale_x_discrete(name="Basis set", limits=c("VDZ-BFD", "VTZ-BFD", "VQZ-BFD"),
                          labels=c("VDZ-BFD", "VTZ-BFD", "VQZ-BFD")
)
p <- p + scale_y_continuous(name = TeX("Number of determinants"),  trans = "log10",
                            breaks = c(1, 10, 100, 1000, 1e4, 1e5, 1e6, 1e7),
                            labels = c("1", "10", "100", "1000", TeX("10^4"), TeX("10^

p <- p + scale_colour_discrete(name = expression(mu),
                               labels = labels)
p <- p + geom_boxplot(varwidth=FALSE,alpha = 1, outlier.shape = 3)
p <- p + geom_point(position = position_dodge(.75), alpha=.2, size=3, stroke=0)
p <- p + theme(text = element_text(size = 20, family="Times"))
```

```
p
```




```
pdf("../Manuscript/g2-ndet.pdf", family="Times", width=16, height=5)
p
dev.off()
```