RSDFT-CIPSI

Anthony Scemama

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Contents

Geometries are given in Angstrom. Basis sets and pseudopotentials are given in GAMESS(US) format.

$$\mu_i \approx \frac{1}{2}\frac{1.5^i}{1.5^3}$$

1 H_2O

Reference atomization energy : 0.371900 au

1.1 XYZ file

Same Geometry as in `doi:10.1063/1.4947093`

```
3
Water from doi:10.1063/1.4947093
O       0.                      0.   0.
H      -0.756950272703377558    0.  -0.585882234512562827
H       0.756950272703377558    0.  -0.585882234512562827
```

Nuclear repulsion energy : 6.983610526929691

1.2 Pseudopotential

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

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
```

1.3 DONE cc-pVDZ-BFD

```
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

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
```

24 AOs, 23 MOs

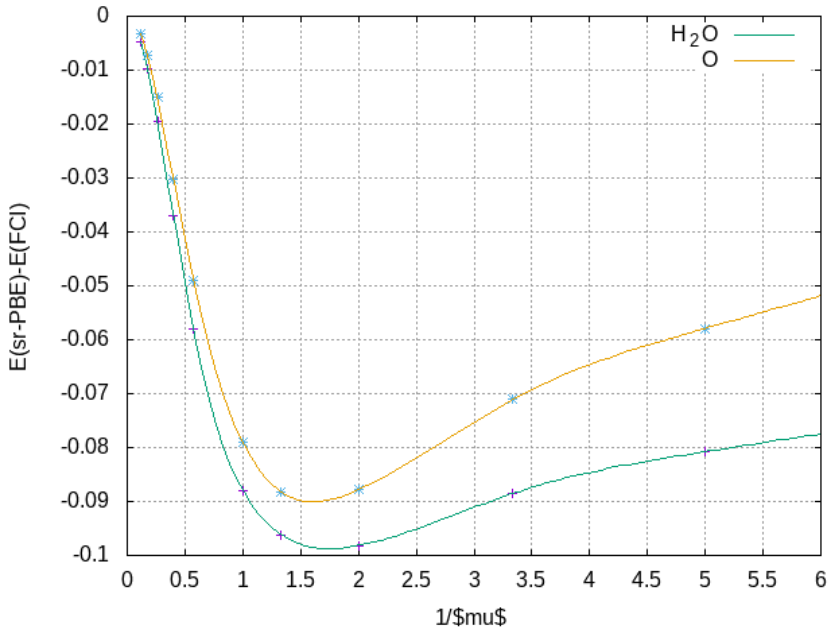
1.3.1 HF energy:

H2O	-16.94804007785208
H	-0.4990452313322324
O	-15.70594174131179

1.3.2 CCSD(T) dissociation energy: 0.333219 au

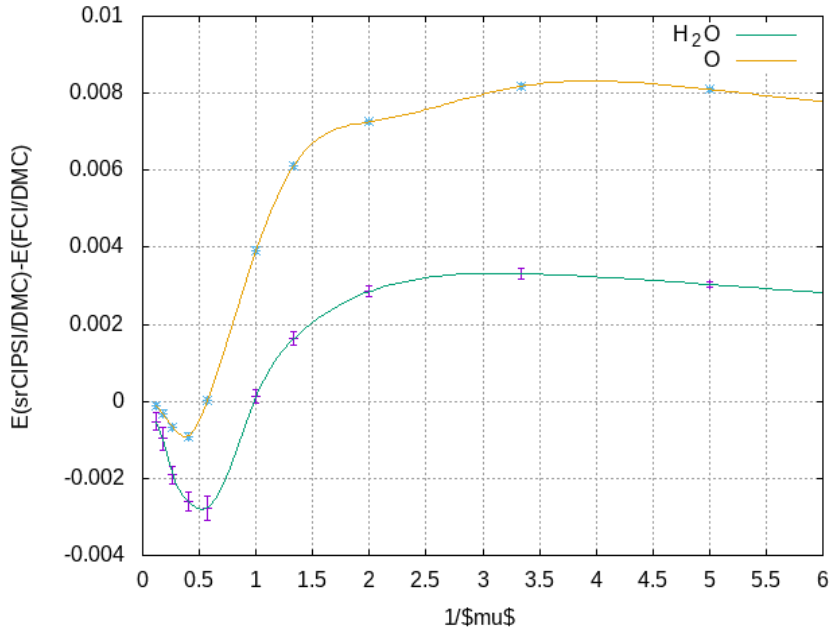
1.3.3 CIPSI with natural orbitals

	H_2O		H		O		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	E_{at}
1. (-6)	11	-17.2464827355670	1	-0.497462910963732	32	-15.8926592152696	0.35
0.20	23	-17.2454472136151	1	-0.497675271883671	18	-15.8906553675359	0.35
0.30	53	-17.2531752249923	1	-0.500020054995876	22	-15.8991860505193	0.35
0.50	1442	-17.2627954176401	1	-0.502301769176686	95	-15.9113115088349	0.34
0.75	3213	-17.2608600031439	1	-0.501902392897537	431	-15.9125649495245	0.34
1.00	6743	-17.2526327790576	1	-0.500915129067989	571	-15.9054097072708	0.34
1.75	54540	-17.2227612803246	1	-0.499556360741909	1064	-15.8778827081260	0.34
2.50	51691	-17.2017620477491	1	-0.499220775536428	1879	-15.8599672611832	0.34
3.80	103059	-17.1841520428494	1	-0.499087178764149	1846	-15.8450343476922	0.34
5.70	102599	-17.1743644569390	1	-0.499054690526038	1944	-15.8372541996167	0.33
8.50	101803	-17.1692969615481	1	-0.499047296040090	1943	-15.8333886253435	0.33
∞	200521	-17.1644196532044	1	-0.49904523	15699	-15.8300247094224	0.33
ExFCI	NA	-17.164669	1	-0.49904523	NA	-15.83002472	0.33



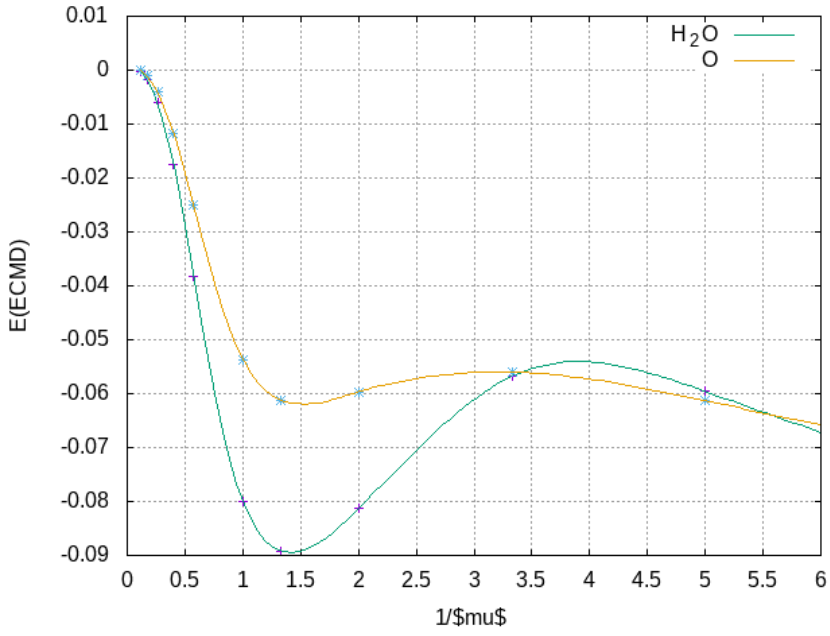
1.3.4 QMC

	H_2O				H			
μ	N_{det}	E(DMC)	Error	N_{det}	E(DMC)	Error	N_{det}	
1. (-6)	11	-17.2535927658	0.0000616883	1	-0.5000010174	0.0000172350	32	-15
0.20	23	-17.2537299553	0.0000673868	1	-0.5000031727	0.0000098305	18	-15
0.30	53	-17.2534524288	0.0001389013	1	-0.5000014039	0.0000201664	22	-15
0.50	1442	-17.2539120512	0.0001475010	1	-0.4999990746	0.0000135287	95	-15
0.75	3213	-17.2551351593	0.0001757492	1	-0.4999704651	0.0000123770	431	-15
1.00	6743	-17.2566320269	0.0001881680	1	-0.4999828909	0.0000123869	571	-15
1.75	54540	-17.2595366309	0.0003193539	1	-0.4999832501	0.0000118522	1064	-15
2.50	51691	-17.2593693798	0.0002564347	1	-0.5000182128	0.0000122194	1879	-15
3.80	103059	-17.2586706893	0.0002222800	1	-0.4999868144	0.0000178879	1846	-15
5.70	102599	-17.2577349871	0.0002927319	1	-0.5000137286	0.0000197492	1944	-15
8.50	101803	-17.2572986405	0.0002283964	1	-0.4999852648	0.0000097121	1943	-15
inf	200521	-17.2567650693	0.0005779960	1	-0.5000103856	0.0000211133	15699	-15



1.3.5 ECMD

	H_2O		H		O		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	$E_{atomization}$
1. (-6)	11	-16.9448707424	1	-0.49904523	32	-15.7028012993	0.24397898
0.20	23	-17.2242666759	1	-0.49904523	18	-15.8913535806	0.33482264
0.30	53	-17.2213647451	1	-0.49904523	22	-15.8860197374	0.33725455
0.50	1442	-17.2460034776	1	-0.49904523	95	-15.8897226418	0.35819038
0.75	3213	-17.2538396234	1	-0.49904523	431	-15.8911624468	0.36458672
1.00	6743	-17.2445547711	1	-0.49904523	571	-15.8836840393	0.36278027
1.75	54540	-17.2028094097	1	-0.49904523	1064	-15.8550921703	0.34962678
2.50	51691	-17.1821264648	1	-0.49904523	1879	-15.8417340743	0.34230193
3.80	103059	-17.1707019945	1	-0.49904523	1846	-15.8339576594	0.33865388
5.70	102599	-17.1663719591	1	-0.49904523	1944	-15.8311365603	0.33714494
8.50	101803	-17.1648836325	1	-0.49904523	1943	-15.8300240953	0.33676908
∞	200521	-17.1644196534	1	-0.49904523	15699	-15.8301288718	0.33620032
ExFCI	NA	-17.164669	1	-0.49904523	NA	-15.83002472	0.33655382



1.4 DONE cc-pVTZ-BFD

```
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

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
```

62 AOs, 55 MOs

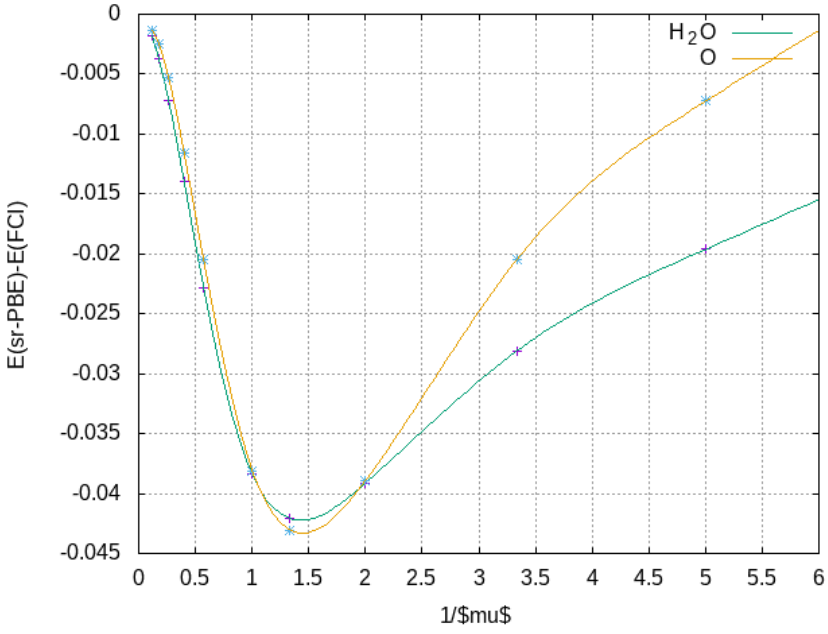
1.4.1 HF energy:

H2O	-16.95323238971265
H	-0.4990429174703885
O	-15.70800126366209

1.4.2 CCSD(T) dissociation energy: 0.359559 au

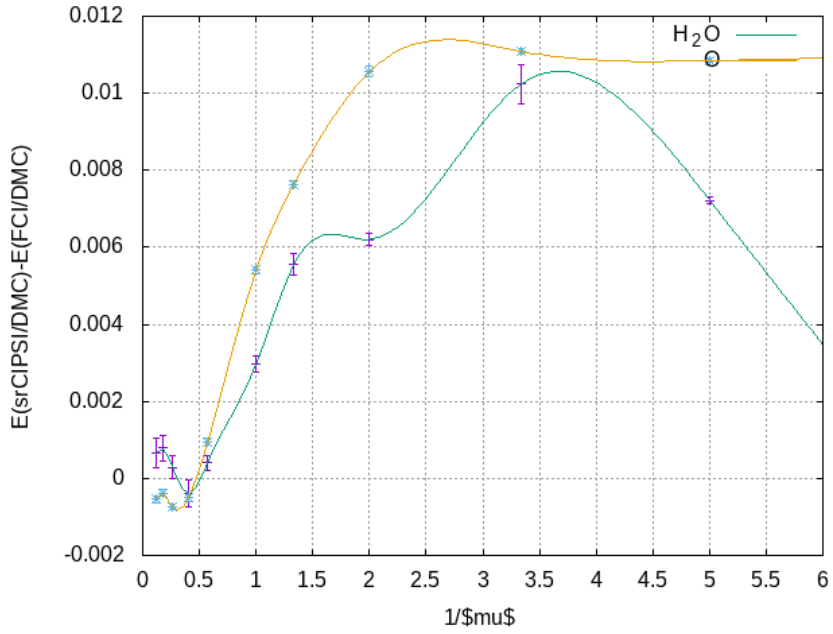
1.4.3 CIPSI with natural orbitals

	H_2O		H		O		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	E
1. (-6)	23	-17.2523870798208	1	-0.497455949623173	56	-15.8943418199011	0
0.20	23	-17.2517850749956	1	-0.497667829593971	44	-15.8925846521328	0
0.30	219	-17.2602989385967	1	-0.500012863167701	44	-15.9011337704962	0
0.50	1699	-17.2712812851578	1	-0.502296128041502	387	-15.9149780380730	0
0.75	13362	-17.2742507881653	1	-0.501898409513286	1133	-15.9199259292212	0
1.00	25673	-17.2705814448750	1	-0.500911996264451	2291	-15.9169272791252	0
1.75	207475	-17.2550176120029	1	-0.499553910797633	9594	-15.9020240076499	0
2.50	858123	-17.2461435031256	1	-0.499218425280479	21911	-15.8938546433323	0
3.80	1621513	-17.2393621693893	1	-0.499084857864629	18329	-15.8877260665965	0
5.70	1629655	-17.2358436456985	1	-0.499052375301986	21941	-15.8850092841849	0
8.50	1643301	-17.2339427191574	1	-0.499044981913016	42217	-15.8838759830564	0
∞	1631982	-17.2316182510754	1	-0.499042917477163	282793	-15.8825637842011	0
ExFCI		-17.23217115		-0.499042917477163		-15.88257866	0



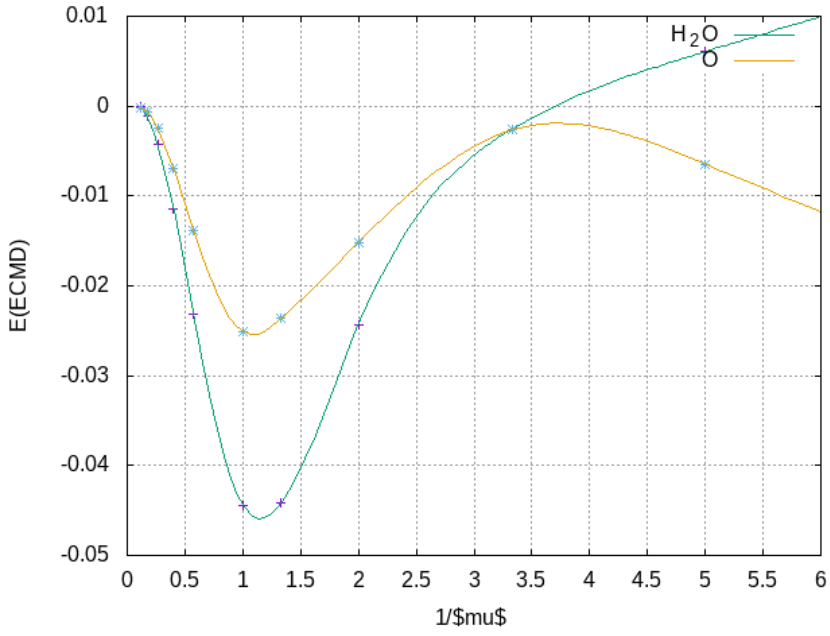
1.4.4 QMC

	H_2O				H			
μ	N_{det}	E(DMC)	Error	N_{det}	E(DMC)	Error	N_{det}	
1. (-6)	11	-17.2567442368	0.0000674814	1	-0.4999898051	0.0000065175	32	-15
0.20	23	-17.2567293499	0.0000806448	1	-0.5000210771	0.0000097491	18	-15
0.30	53	-17.2537172349	0.0005108024	1	-0.4999868887	0.0000149003	22	-15
0.50	1442	-17.2577489156	0.0001590032	1	-0.4999987389	0.0000138110	95	-15
0.75	3213	-17.2583975528	0.0002828675	1	-0.5000191125	0.0000109315	431	-15
1.00	6743	-17.2609826285	0.0002158278	1	-0.4999862089	0.0000119766	571	-15
1.75	54540	-17.2635480054	0.0001864936	1	-0.4999666515	0.0000131903	1064	-15
2.50	51691	-17.2643468817	0.0003484087	1	-0.4999801617	0.0000094324	1879	-15
3.80	103059	-17.2636697373	0.0002950991	1	-0.5000085861	0.0000085475	1846	-15
5.70	102599	-17.2631675892	0.0003358884	1	-0.5000055184	0.0000147803	1944	-15
8.50	101803	-17.2632963114	0.0003799317	1	-0.5000010336	0.0000123807	1943	-15
inf	200521	-17.2638832283	0.0002702253	1	-0.4999916320	0.0000135918	15699	-15



1.4.5 ECMD

	H_2O		H		O		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	$E_{atomization}$
1. (-6)	23	-16.9474227226	1	-0.4990429175	56	-15.7018131902	0.24752370
0.20	23	-17.2261065833	1	-0.4990429175	44	-15.8890274854	0.33899326
0.30	219	-17.2347208976	1	-0.4990429175	44	-15.8852236174	0.35141145
0.50	1699	-17.2565233809	1	-0.4990429175	387	-15.8977227918	0.36071475
0.75	13362	-17.2763408603	1	-0.4990429175	1133	-15.9062325977	0.37202243
1.00	25673	-17.2765522162	1	-0.4990429175	2291	-15.9076662553	0.37080013
1.75	207475	-17.2553166617	1	-0.4990429175	9594	-15.8963737107	0.36085712
2.50	858123	-17.2436535008	1	-0.4990429175	21911	-15.8895990392	0.35596863
3.80	1621513	-17.2363656023	1	-0.4990429175	18329	-15.8850079618	0.35327181
5.70	1629655	-17.2333460576	1	-0.4990429175	21941	-15.8832438185	0.35201640
8.50	1643301	-17.2322131312	1	-0.4990429175	42217	-15.8827440572	0.35138324
∞	1631982	-17.2316182511	1	-0.4990429175	282793	-15.8825637842	0.35096863
ExFCI		-17.23217115		-0.4990429175		-15.88257866	0.35150666



1.4.6 Analyzis of coefficients

cannot open the connection

1.5 TODO cc-pVQZ-BFD

```
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

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
```

139 AOs, 114 MOs

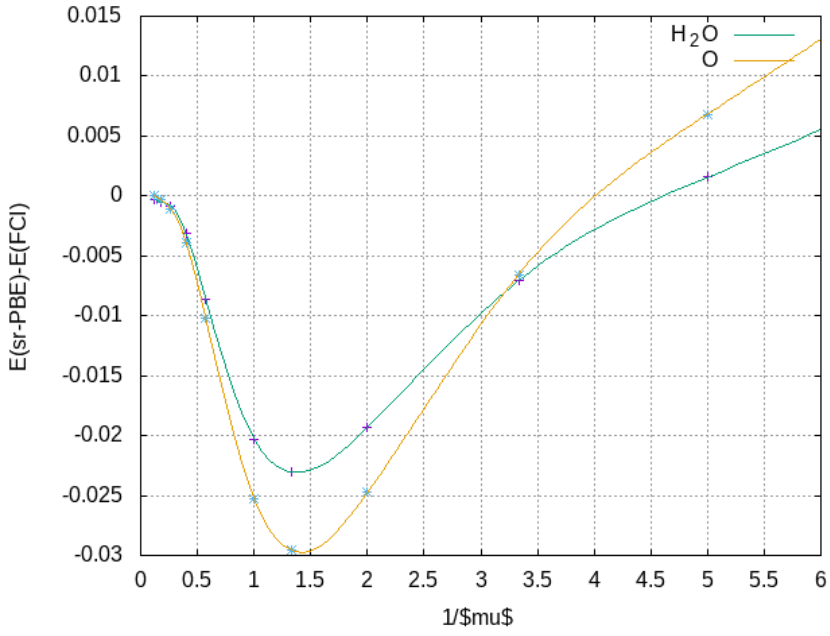
1.5.1 HF energy:

H2O	-16.95323238971265
H	-0.4999159485752356
O	-15.70838239857190

1.5.2 CCSD(T) dissociation energy: ??? au

1.5.3 CIPSI with natural orbitals

	H_2O		H		O	
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)
1. (-6)	23	-17.2550713148646	1	-0.498770397586525	41	-15.8945440099478
0.20	23	-17.2544983309796	1	-0.498943556678728	39	-15.8927491298105
0.30	214	-17.2631125033426	1	-0.501238867081562	88	-15.9015447645282
0.50	3355	-17.2753425267816	1	-0.503289490954576	369	-15.9156299499914
0.75	24685	-17.2791002023973	1	-0.502729685060127	2152	-15.9216014051348
1.00	51016	-17.2763349199718	1	-0.501722057158799	4324	-15.9193017992612
1.75	832153	-17.2646439398390	1	-0.500400995599045	14431	-15.9068519442068
2.50	1657867	-17.2591970797300	1	-0.500081369220756	30186	-15.9011704544825
3.80	3393009	-17.2568806209183	1	-0.499955311987831	94180	-15.8985952759131
5.70	6849236	-17.2565805594566	1	-0.499924811823201	101131	-15.8978811997698
8.50	6501453	-17.2563271562921	1	-0.499917882290281	94108	-15.8976152329438
∞	6555322	-17.2555127230293	1	-0.499915948575730	1614219	-15.8976190012628
ExFCI		-17.25606450		-0.499915948575730		-15.89763971



2 C_2

Data taken from `doi:10.1021/ct300504f` Reference atomization energy : 146.9(5) kcal/mol = 0.2341(8) au

2.1 XYZ file

Same Geometry as in doi:10.1021/ct300504f

```
2
C2
C       0.   0.  -0.62125
C       0.   0.   0.62125
```

Nuclear repulsion energy : 6.814354426334003

2.2 Pseudopotential

```
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
```

2.2.1 cc-pVDZ-BFD

```
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
```

28 AOs, 26 MOs

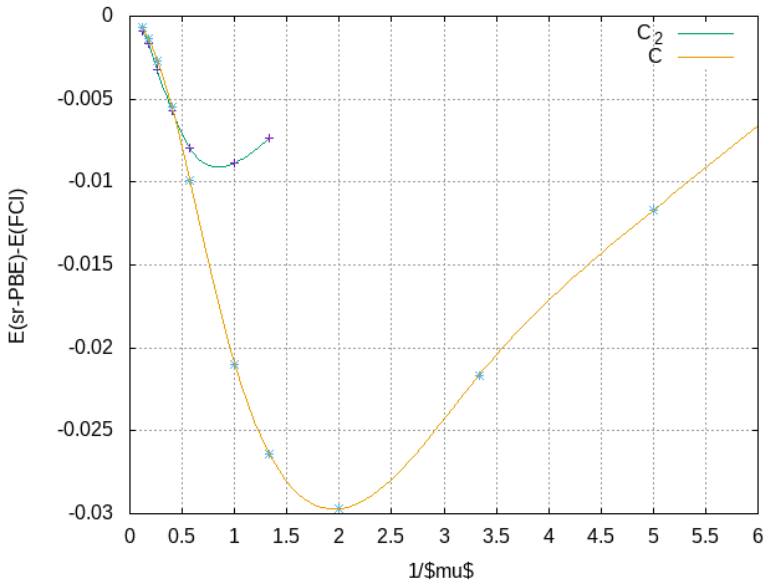
1. HF energy:

C2	-10.67893455005543
C	-5.328989707682060

2. i-FCIQMC dissociation energy: 129.95(8) kcal/mol = 0.2071(1) au

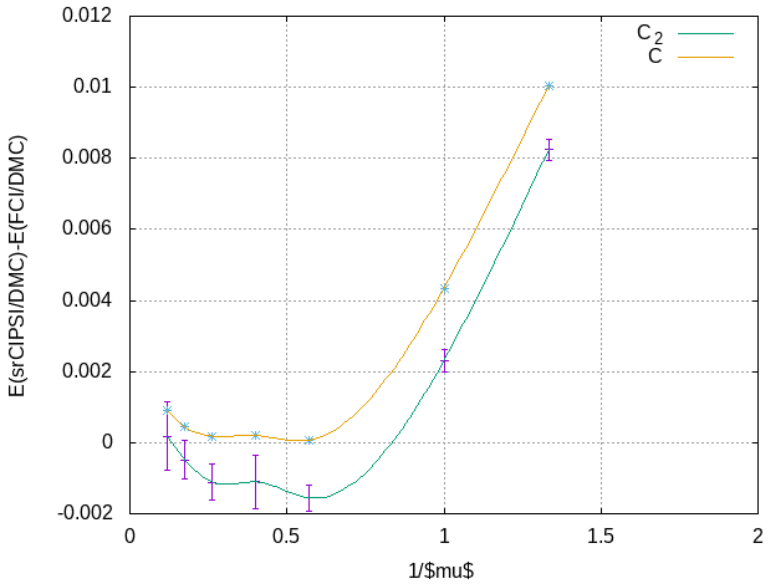
3. CIPSI with natural orbitals

	C_2		C		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	$E_{atomization}$
1. (-6)	NA	NA	22	-5.41505706988073	-10.830114
0.20	NA	NA	9	-5.41545184840256	-10.830904
0.30	NA	NA	21	-5.42042892115798	-10.840858
0.50	NA	NA	135	-5.42445651484712	-10.848913
0.75	52960	-11.0308445085580	163	-5.42281416310061	0.18521618
1.00	104403	-11.0323357336759	330	-5.42008673295876	0.19216227
1.75	408078	-11.0314245120875	509	-5.41456475332999	0.20229501
2.50	822205	-11.0291998069478	513	-5.41233203015442	0.20453575
3.80	703001	-11.0267092471890	511	-5.41095120348554	0.20480684
5.70	715415	-11.0251197032813	498	-5.41028104327860	0.20455762
8.50	1421782	-11.0243736638120	498	-5.40994218754541	0.20448929
∞	722672	-11.0229208360228	498	-5.40958049910186	0.20375984
ExFCI	NA	-11.02347855		-5.40960365	0.20427125



4. QMC

	C_2			C			
μ	N_{det}	E(DMC)	Error	N_{det}	E(DMC)	Error	
1.(-6)	NA	NA	NA	22	-5.4167052434	0.0000222156	-10.8
0.20	NA	NA	NA	9	-5.4165906853	0.0000221124	-10.8
0.30	NA	NA	NA	21	-5.4188382207	0.0000229444	-10.8
0.50	NA	NA	NA	135	-5.4223620093	0.0000352887	-10.8
0.75	52960	-11.0824209839	0.0002919653	163	-5.4269017472	0.0000303835	
1.00	104403	-11.0883588662	0.0003090548	330	-5.4297546085	0.0000282413	
1.75	408078	-11.0922216603	0.0003714282	509	-5.4319232617	0.0000273252	
2.50	822205	-11.0917742794	0.0007445867	513	-5.4320468517	0.0000326056	
3.80	703001	-11.0917756277	0.0005178753	511	-5.4319428879	0.0000258094	
5.70	715415	-11.0911492931	0.0005317107	498	-5.4318199101	0.0000282036	
8.50	1421782	-11.0904822882	0.0009636942	498	-5.4318044503	0.0000339472	
inf	722672	-11.0906232109	0.0004176631	498	-5.4317735738	0.0000258448	



5. Analyzis of coefficients

cannot open the connection

2.2.2 cc-pVTZ-BFD

```
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
```

68 AOs, 58 MOs

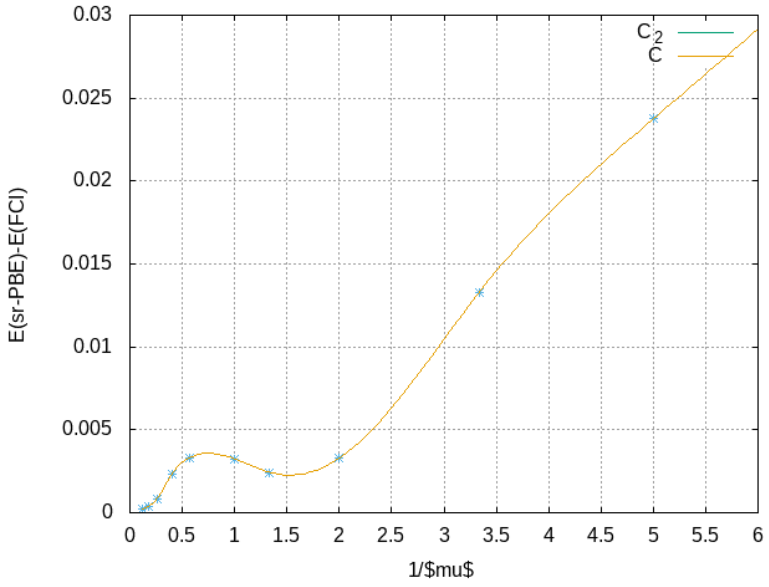
1. HF energy:

C2
C

2. i-FCIQMC dissociation energy: 139.69(8) kcal/mol = 0.2226(1) au

3. CIPSI with natural orbitals

	C_2		C		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	$E_{atomization}$
1. (-6)	NA	NA	17	-5.41553696548016	-10.831074 - NA
0.20	NA	NA	17	-5.41613005236001	-10.832260 - NA
0.30	NA	NA	38	-5.42137104699040	-10.842742 - NA
0.50	NA	NA	138	-5.42636764143841	-10.852735 - NA
0.75	NA	NA	270	-5.42679122653394	-10.853582 - NA
1.00	NA	NA	528	-5.42639163352912	-10.852783 - NA
1.75	NA	NA	1077	-5.42634487557905	-10.852690 - NA
2.50	NA	NA	1034	-5.42684001117528	-10.853680 - NA
3.80	NA	NA	2172	-5.42757813990369	-10.855156 - NA
5.70	NA	NA	2160	-5.42782845289081	-10.855657 - NA
8.50	NA	NA	2166	-5.42790762317720	-10.855815 - NA
∞	722672	NA	2156	-5.42791084828515	-10.855822 - NA
ExFCI	NA	-11.02343265		-5.42800915	0.16741435



2.2.3 cc-pVQZ-BFD

```
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
```

138 AOs, _ MOs HF energy:

1. HF energy:

   C2
   C

2. CCSD(T) dissociation energy: ??? au

3. CIPSI with natural orbitals

	C_2		C		
μ	N_{det}	E(CIPSI)	N_{det}	E(CIPSI)	$E_{atomization}$
1. (-6)					0.
0.20					0.
0.30					0.
0.50					0.
0.75					0.
1.00					0.
1.75					0.
2.50					0.
3.80					0.
5.70					0.
8.50					0.
∞	722672				0.
ExFCI	NA	-11.02343265		-5.40960365	0.20422535

2.3 G2, $\mu = 1/2$

2.3.1 FCI avec extrapolation

2.3.2 FCI avec mu=0.5, mu=1.0

3 G2

Determinant localization approximation J. Chem. Phys. 151, 134105 (2019); https://doi.org/10.1063/1.5119729

3.1 pVDZ, BFD

NaCl and BeH removed because of pseudopotential instabilities in QMC

3.1.1 CCSD(T)/cc-pVDZ : 22.89

3.1.2 TODO CCSD(T)/VDZ-BFD :

3.1.3 PBE0/VDZ-BFD : 11.38

3.1.4 DONE $\mu = 0$

1. CIPSI
   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.993248			
C	-5.415055			
Cl	-14.939962			
F	-24.186526			
H	-0.497467			
Li	-0.200658			
N	-9.781514			
Na	-0.022632			
O	-15.892648			
P	-6.462366			
S	-10.108549			
Si	-3.762685			
BeH	-1.558892	0.068177	0.079400	-7.042813
C2H2	-12.471755	0.646709	0.642400	2.704245
C2H4	-13.725077	0.905097	0.899000	3.826163
C2H6	-14.956921	1.142007	1.136900	3.204438
$CH2_{1A1}$	-6.693763	0.283774	0.288900	-3.216921
$CH2_{3B1}$	-6.717840	0.307850	0.304100	2.352985
CH3	-7.400854	0.493396	0.490800	1.629309
CH3Cl	-22.481099	0.633680	0.631000	1.681825
CH4	-8.076189	0.671265	0.670300	0.605321
CH	-6.046751	0.134228	0.133900	0.205939
Cl2	-29.973622	0.093699	0.094000	-0.189045
ClF	-39.225341	0.098854	0.100100	-0.782028
ClO	-30.939725	0.107115	0.104700	1.515226
CN	-15.442585	0.246016	0.288800	-26.847116
CO	-21.720796	0.413093	0.413700	-0.381048
CO2	-37.836720	0.636369	0.621400	9.393025
CS	-15.798392	0.274788	0.274000	0.494574
F2	-48.441597	0.068546	0.062200	3.982102
H2CO	-22.906458	0.603820	0.596700	4.468077
H2O	-17.246706	0.359123	0.371900	-8.017457
H2O2	-33.202083	0.421852	0.429400	-4.736392
H2S	-11.389764	0.286281	0.292000	-3.588781
H3COH	-24.114576	0.817003	0.818700	-1.064732
H3CSH	-18.268126	0.754653	0.757000	-1.473010
HCl	-15.604810	0.167381	0.171000	-2.271269
HCN	-16.198541	0.504504	0.496900	4.771874
HCO	-22.259685	0.454514	0.444700	6.158611
HF	-24.897718	0.213725	0.226100	-7.765617
HOCl	-31.590638	0.260560	0.264700	-2.597620
Li2	-0.428520	0.027205	0.038900	-7.338974
LiF	-24.594032	0.206849	0.222000	-9.507551
LiH	-0.782772	0.084647	0.092430	-4.883785
N2	-19.930508	0.367480	0.364600	1.807460
N2H4	-22.248736	0.695840	0.699600	-2.359744
Na2	-0.388095	0.342830	0.026800	198.312096

(b) MAD = 10.08

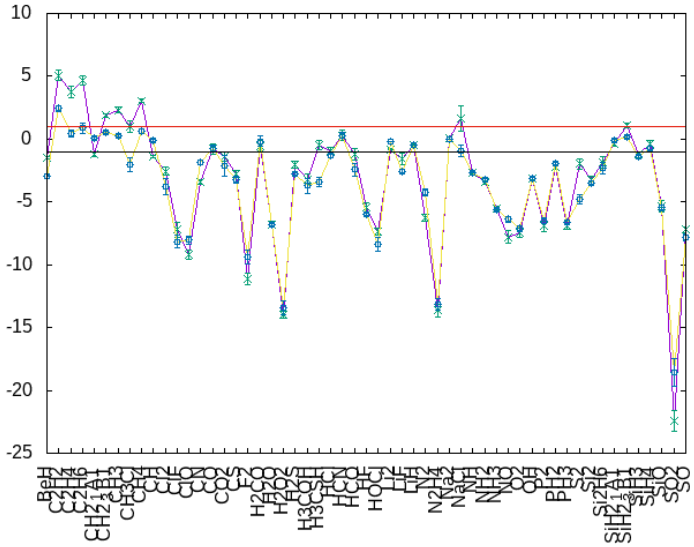
2. QMC with Jastrow

(a) Table

	Total E Hartree	Delta E Hartree			Reference Hartree	Error kcal/mol	
Be	-0.998195	0.000084	0.000000	0.000119			
C	-5.416566	0.000150	0.000000	0.000213			
Cl	-14.941245	0.000447	0.000000	0.000632			
F	-24.189403	0.000284	0.000000	0.000401			
H	-0.500022	0.000016	0.000000	0.000023			
Li	-0.196328	0.000010	0.000000	0.000015			
N	-9.788652	0.000184	0.000000	0.000261			
Na	-0.182137	0.000007	0.000000	0.000009			
O	-15.893004	0.000249	0.000000	0.000351			
P	-6.462677	0.000178	0.000000	0.000251			
S	-10.109875	0.000259	0.000000	0.000367			
Si	-3.758652	0.000155	0.000000	0.000219			
BeH	-1.577113	0.000136	0.078896	0.000161	0.079400	-0.316081	0.101037
C2H2	-12.484306	0.000544	0.651129	0.000622	0.642400	5.477726	0.390311
C2H4	-13.738603	0.000925	0.905381	0.000975	0.899000	4.004129	0.611816
C2H6	-14.980663	0.000903	1.147396	0.000957	1.136900	6.586444	0.600403
$CH2_{1A1}$	-6.702902	0.000274	0.286291	0.000314	0.288900	-1.637004	0.197212
$CH2_{3B1}$	-6.725283	0.000288	0.308672	0.000326	0.304100	2.868731	0.204805
CH3	-7.411669	0.000364	0.495036	0.000397	0.490800	2.657913	0.249214
CH3Cl	-22.490031	0.000909	0.632153	0.001025	0.631000	0.723298	0.643303
CH4	-8.092553	0.000363	0.675897	0.000399	0.670300	3.511964	0.250151
CH	-6.049161	0.000205	0.132572	0.000255	0.133900	-0.833098	0.160006
Cl2	-29.971055	0.000733	0.088565	0.001156	0.094000	-3.410271	0.725335
ClF	-39.218604	0.000684	0.087957	0.000865	0.100100	-7.620100	0.542541
ClO	-30.923695	0.000772	0.089446	0.000926	0.104700	-9.572074	0.580869
CN	-15.440439	0.000769	0.235221	0.000805	0.288800	-33.621405	0.505013
CO	-21.720503	0.000492	0.410932	0.000571	0.413700	-1.736715	0.358251
CO2	-37.823903	0.000944	0.621328	0.001078	0.621400	-0.045019	0.676306
CS	-15.791740	0.000480	0.265299	0.000566	0.274000	-5.460020	0.354871
F2	-48.422635	0.000687	0.043830	0.000891	0.062200	-11.527266	0.559416
H2CO	-22.906324	0.000575	0.596709	0.000645	0.596700	0.005546	0.404853
H2O	-17.253507	0.000320	0.360458	0.000406	0.371900	-7.179990	0.254913
H2O2	-33.193945	0.000760	0.407892	0.000909	0.429400	-13.496719	0.570445
H2S	-11.395515	0.000391	0.285594	0.000471	0.292000	-4.019632	0.295274
H3COH	-24.125862	0.000882	0.816201	0.000931	0.818700	-1.567895	0.584320
H3CSH	-18.279519	0.000852	0.752988	0.000905	0.757000	-2.517762	0.568093
HCl	-15.610321	0.000350	0.169054	0.000568	0.171000	-1.221384	0.356469
HCN	-16.202249	0.000494	0.497008	0.000549	0.496900	0.067993	0.344280
HCO	-22.250594	0.000512	0.441001	0.000589	0.444700	-2.321031	0.369470
HF	-24.906363	0.000324	0.216938	0.000431	0.226100	-5.749100	0.270501
HOCl	-31.585137	0.000768	0.250865	0.000922	0.264700	-8.681338	0.578818
Li2	-0.427804	0.000071	0.035147	0.000074	0.038900	-2.354765	0.046550
LiF	-24.605221	0.000310	0.219490	0.000421	0.222000	-1.575114	0.263918
LiH	-0.787749	0.000088	0.091399	0.000090	0.092430	-0.647208	0.056310
N2	-19.929286	0.000488	0.351981	0.000612	0.364600	-7.918621	0.383837
N2H4	-22.255566	0.000807	0.678171	0.000890	0.699600	-13.446931	0.558545
Na2	-0.391093	0.000083	0.026819	0.000084	0.026800	0.011832	0.052871

(b) MAD = 5.07 +/- 0.44

(c) Figure



3.1.5 DONE $\mu = 1/4$

1. CIPSI

   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.990898			
C	-5.418170			
Cl	-14.937611			
F	-24.188208			
H	-0.498899			
Li	-0.198788			
N	-9.786270			
Na	-0.176097			
O	-15.894795			
P	-6.461580			
S	-10.106026			
Si	-3.759767			
BeH	-1.558909	0.069111	0.079400	-6.456475
C2H2	-12.471698	0.637560	0.642400	-3.037220
C2H4	-13.726706	0.894768	0.899000	-2.655519
C2H6	-14.962823	1.133087	1.136900	-2.392704
$CH2_{1A1}$	-6.693768	0.277799	0.288900	-6.966033
$CH2_{3B1}$	-6.720192	0.304223	0.304100	0.077471
CH3	-7.402377	0.487509	0.490800	-2.065178
CH3Cl	-22.479630	0.627151	0.631000	-2.415124
CH4	-8.077764	0.663997	0.670300	-3.955332
CH	-6.046905	0.129835	0.133900	-2.550684
Cl2	-29.964137	0.088916	0.094000	-3.190568
ClF	-39.223298	0.097479	0.100100	-1.644539
ClO	-30.934485	0.102079	0.104700	-1.644598
CN	-15.489681	0.285241	0.288800	-2.233465
CO	-21.724108	0.411144	0.413700	-1.604169
CO2	-37.837557	0.629798	0.621400	5.269703
CS	-15.789705	0.265510	0.274000	-5.327873
F2	-48.443178	0.066763	0.062200	2.863228
H2CO	-22.908464	0.597700	0.596700	0.627571
H2O	-17.249751	0.357158	0.371900	-9.250928
H2O2	-33.205714	0.418325	0.429400	-6.949513
H2S	-11.384757	0.280933	0.292000	-6.944801
H3COH	-24.120733	0.812171	0.818700	-4.097129
H3CSH	-18.266078	0.746285	0.757000	-6.723789
HCl	-15.601020	0.164510	0.171000	-4.072465
HCN	-16.198560	0.495220	0.496900	-1.054027
HCO	-22.261161	0.449297	0.444700	2.884545
HF	-24.900836	0.213729	0.226100	-7.763223
HOCl	-31.588728	0.257423	0.264700	-4.566233
Li2	-0.427271	0.029694	0.038900	-5.776626
LiF	-24.598963	0.211967	0.222000	-6.295769
LiH	-0.784367	0.086680	0.092430	-3.608453
N2	-19.931576	0.359035	0.364600	-3.491877
N2H4	-22.254132	0.685994	0.699600	-8.537908
Na2	-0.384111	0.031918	0.026800	3.211375

(b) MAD = 5.55

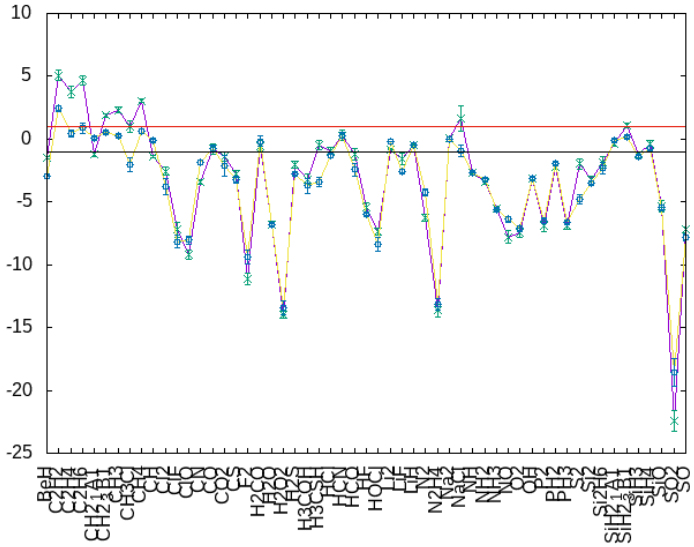
2. QMC with Jastrow

(a) Table

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
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
C2H4	-13.741231	0.000683	0.905014	0.000733	0.899000	3.773550	0.460116
C2H6	-14.980526	0.000464	1.144325	0.000543	1.136900	4.659101	0.340885
$CH2_{1A1}$	-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
CH4	-8.093244	0.000174	0.675152	0.000231	0.670300	3.044423	0.144710
CH	-6.049806	0.000150	0.131689	0.000197	0.133900	-1.387389	0.123828
Cl2	-29.973351	0.000494	0.089927	0.000545	0.094000	-2.555890	0.341684
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
CN	-15.490160	0.000308	0.283368	0.000351	0.288800	-3.408539	0.220358
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
CS	-15.796844	0.000377	0.269651	0.000426	0.274000	-2.728813	0.267315
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
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
H3COH	-24.124458	0.000636	0.813580	0.000678	0.818700	-3.212607	0.425360
H3CSH	-18.283433	0.000546	0.756272	0.000587	0.757000	-0.456731	0.368206
HCl	-15.611220	0.000442	0.169515	0.000457	0.171000	-0.931623	0.287064
HCN	-16.204158	0.000579	0.497375	0.000603	0.496900	0.297906	0.378384
HCO	-22.253647	0.000678	0.442745	0.000713	0.444700	-1.226619	0.447521
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
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
Na2	-0.391001	0.000066	0.026926	0.000081	0.026800	0.079339	0.051089

(b) MAD = 4.04 +/- 0.37

(c) Figure



3.1.6 DONE $\mu = 1/2$

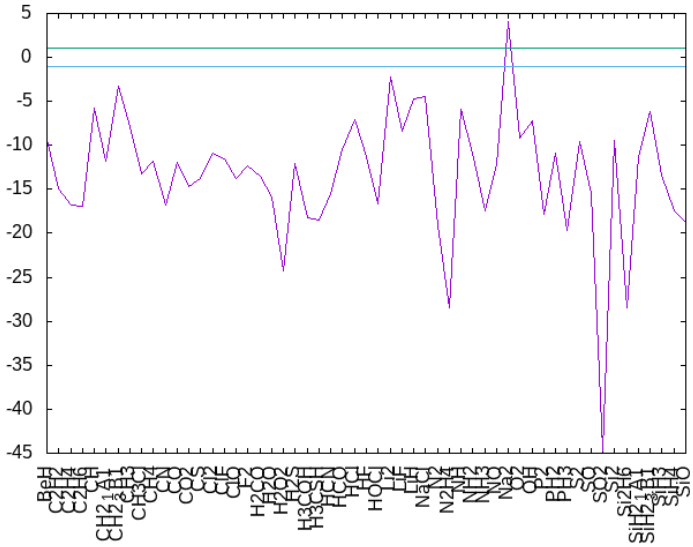
1. CIPSI

   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.992733			
C	-5.424193			
Cl	-14.936917			
F	-24.211164			
H	-0.502302			
Li	-0.196387			
N	-9.800001			
Na	-0.174540			
O	-15.911458			
P	-6.459292			
S	-10.103616			
Si	-3.755570			
BeH	-1.559665	0.064630	0.079400	-9.268590
C2H2	-12.471534	0.618546	0.642400	-14.968783
C2H4	-13.729919	0.872327	0.899000	-16.737595
C2H6	-14.972133	1.109937	1.136900	-16.919464
CH	-6.051231	0.124737	0.133900	-5.750116
$CH2_{1A1}$	-6.698845	0.270049	0.288900	-11.829303
$CH2_{3B1}$	-6.727757	0.298961	0.304100	-3.224773
CH3	-7.409416	0.478319	0.490800	-7.832194
CH3Cl	-22.477835	0.609820	0.631000	-13.290489
CH4	-8.084849	0.651450	0.670300	-11.828671
CN	-15.486349	0.262155	0.288800	-16.719820
CO	-21.730324	0.394674	0.413700	-11.939218
CO2	-37.845033	0.597923	0.621400	-14.731778
CS	-15.779785	0.251977	0.274000	-13.819555
Cl2	-29.950545	0.076711	0.094000	-10.848822
ClF	-39.229805	0.081725	0.100100	-11.530775
ClO	-30.931179	0.082804	0.104700	-13.740165
F2	-48.464871	0.042543	0.062200	-12.334916
H2CO	-22.915457	0.575202	0.596700	-13.490053
H2O	-17.262607	0.346545	0.371900	-15.910229
H2O2	-33.218344	0.390824	0.429400	-24.206976
H2S	-11.381054	0.272835	0.292000	-12.026395
H3COH	-24.134504	0.789646	0.818700	-18.231622
H3CSH	-18.264445	0.727429	0.757000	-18.556005
HCN	-16.198797	0.472302	0.496900	-15.435639
HCO	-22.265861	0.427908	0.444700	-10.537012
HCl	-15.598913	0.159695	0.171000	-7.094202
HF	-24.921651	0.208185	0.226100	-11.241954
HOCl	-31.588809	0.238132	0.264700	-16.671508
Li2	-0.428159	0.035385	0.038900	-2.205628
LiF	-24.616249	0.208698	0.222000	-8.347308
LiH	-0.783586	0.084897	0.092430	-4.726728
NaCl	-15.261719	0.150263	0.157400	-4.478848
N2	-19.934126	0.334123	0.364600	-19.124792
N2H4	-22.263550	0.654340	0.699600	-28.400957

(b) MAD = 13.42

(c) Figure



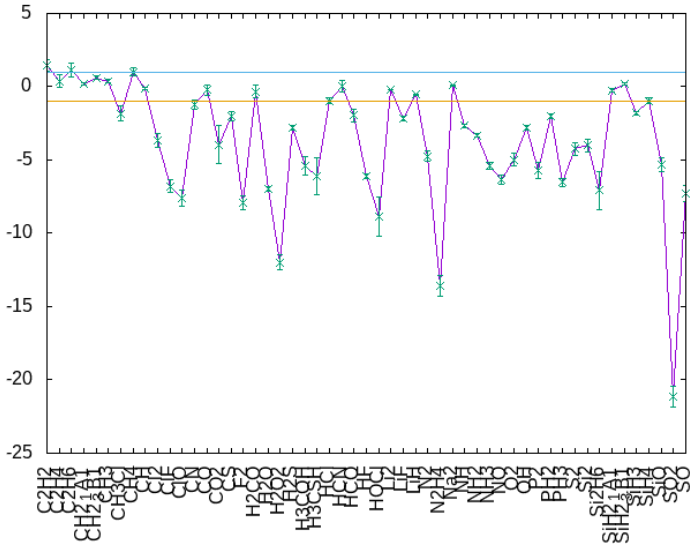
2. QMC without Jastrow

(a) Table

	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
$CH2_{1A1}$	-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
CH	-6.056035	0.000123	0.133695	0.000138	0.133900	-0.128821	0.086597
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
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
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
HCl	-15.619019	0.000217	0.169451	0.000298	0.171000	-0.971823	0.186909
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
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
Na2	-0.391012	0.000017	0.026941	0.000032	0.026800	0.088254	0.020137
NH	-10.418918	0.000163	0.129239	0.000189	0.133500	-2.673761	0.118450

(b) MAD = 3.9 +/- 0.5

(c) Figure



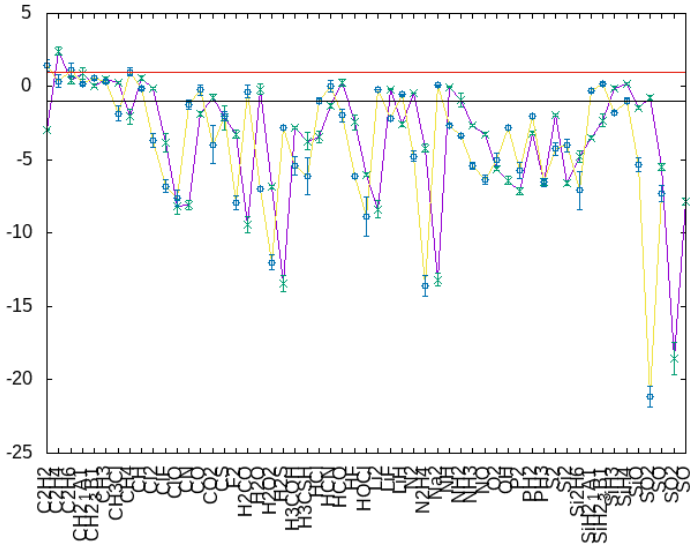
3. QMC with Jastrow

(a) Table

	Total E Hartree		Delta E Hartree		Ref	Error kcal/mol	
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
C2H4	-13.744599	0.000444	0.899725	0.000466	0.899000	0.455073	0.292715
C2H6	-14.983176	0.000623	1.138311	0.000640	1.136900	0.885531	0.401733
$CH2_{1A1}$	-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
CH3	-7.413712	0.000127	0.491280	0.000147	0.490800	0.301192	0.092205
CH3Cl	-22.499891	0.000809	0.627770	0.000817	0.631000	-2.026712	0.512703
CH4	-8.093698	0.000266	0.671270	0.000276	0.670300	0.608405	0.173340
CH	-6.056197	0.000083	0.133756	0.000109	0.133900	-0.090328	0.068429
Cl2	-29.987339	0.000995	0.087961	0.001010	0.094000	-3.789372	0.633674
ClF	-39.225577	0.000775	0.087074	0.000788	0.100100	-8.174187	0.494734
ClO	-30.934845	0.000499	0.091871	0.000511	0.104700	-8.050392	0.320560
CN	-15.497971	0.000251	0.285850	0.000272	0.288800	-1.851206	0.170797
CO	-21.728259	0.000361	0.412527	0.000373	0.413700	-0.735981	0.234286
CO2	-37.827070	0.001289	0.618053	0.001297	0.621400	-2.100522	0.813791
CS	-15.807213	0.000434	0.268826	0.000446	0.274000	-3.246664	0.279694
F2	-48.424857	0.000827	0.047228	0.000857	0.062200	-9.394885	0.538069
H2CO	-22.912166	0.000600	0.596443	0.000608	0.596700	-0.161127	0.381237
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
H2S	-11.403508	0.000134	0.287577	0.000153	0.292000	-2.775745	0.096133
H3COH	-24.128469	0.000930	0.812755	0.000936	0.818700	-3.730536	0.587170
H3CSH	-18.289905	0.000597	0.751536	0.000607	0.757000	-3.428421	0.380612
HCl	-15.618568	0.000238	0.168884	0.000254	0.171000	-1.328058	0.159119
HCN	-16.209503	0.000366	0.497386	0.000382	0.496900	0.305097	0.239420
HCO	-22.256546	0.000832	0.440819	0.000838	0.444700	-2.435571	0.525542
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
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
N2H4	-22.257960	0.000674	0.678627	0.000693	0.699600	-13.161038	0.434984
Na2	-0.391068	0.000018	0.026796	0.000024	0.026800	-0.002375	0.015169

(b) MAD = 3.74 +/- 0.35

(c) Figure



3.1.7 TODO $\mu = 1$

1. CIPSI

   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.997611			
C	-5.420006			
Cl	-14.923700			
F	-24.213585			
H	-0.500915			
Li	-0.195702			
N	-9.797528			
Na	-0.174255			
O	-15.905353			
P	-6.454169			
S	-10.093127			
Si	-3.752249			
BeH	-1.556311	0.057785	0.079400	-13.563652
C2H2	-12.457919	0.616077	0.642400	-16.518135
C2H4	-13.713486	0.869814	0.899000	-18.314755
C2H6	-14.952030	1.106528	1.136900	-19.058990
$CH2_{1A1}$	-6.693312	0.271476	0.288900	-10.933550
$CH2_{3B1}$	-6.719689	0.297853	0.304100	-3.920345
CH3	-7.400261	0.477510	0.490800	-8.339553
CH3Cl	-22.453467	0.607016	0.631000	-15.050240
CH4	-8.076058	0.652392	0.670300	-11.237459
CH	-6.045004	0.124083	0.133900	-6.160218
Cl2	-29.919364	0.071964	0.094000	-13.828005
ClF	-39.205454	0.068169	0.100100	-20.037087
ClO	-30.900816	0.071763	0.104700	-20.668394
CN	-15.473830	0.256296	0.288800	-20.396634
CO	-21.713154	0.387795	0.413700	-16.255639
CO2	-37.813665	0.582952	0.621400	-24.126272
CS	-15.764849	0.251716	0.274000	-13.983341
F2	-48.446924	0.019754	0.062200	-26.635101
H2CO	-22.894495	0.567305	0.596700	-18.445616
H2O	-17.252592	0.345408	0.371900	-16.623808
H2O2	-33.189337	0.376800	0.429400	-33.006901
H2S	-11.368755	0.273798	0.292000	-11.421902
H3COH	-24.111642	0.782622	0.818700	-22.639454
H3CSH	-18.240701	0.723907	0.757000	-20.765895
HCl	-15.586327	0.161712	0.171000	-5.828337
HCN	-16.182131	0.463682	0.496900	-20.844565
HCO	-22.244739	0.418464	0.444700	-16.463310
HF	-24.920723	0.206223	0.226100	-12.472870
HOCl	-31.558798	0.228829	0.264700	-22.509312
Li2	-0.428740	0.037335	0.038900	-0.981967
LiF	-24.610269	0.200982	0.222000	-13.189002
NaCl	-15.245074	0.147118	0.157400	-6.451842
LiH	-0.780131	0.083514	0.092430	-5.595016
N2	-19.913827	0.318770	0.364600	-28.758523
N2H4	-22.236209	0.637492	0.699600	-38.973422

(b) MAD = 17.07

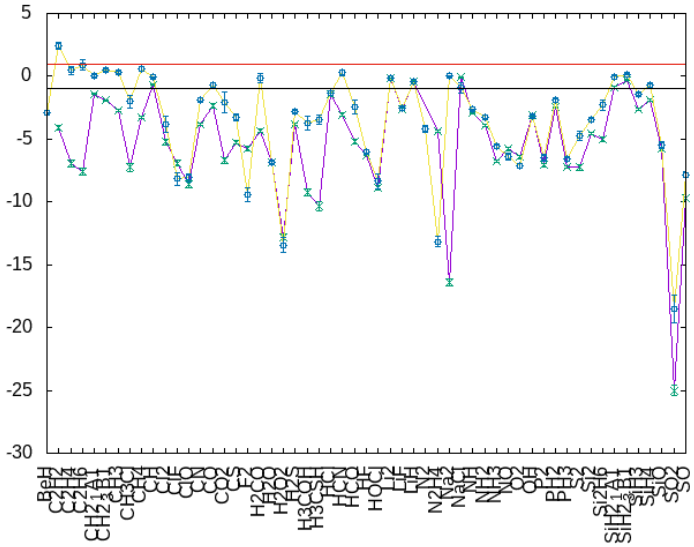
2. QMC with Jastrow

(a) Table

	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							
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
C2H6	-14.983968	0.000387	1.124832	0.000412	1.136900	-7.572876	0.258278
$CH2_{1A1}$	-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
CH4	-8.094626	0.000167	0.665074	0.000189	0.670300	-3.279230	0.118604
CH	-6.062427	0.000050	0.132827	0.000063	0.133900	-0.673247	0.039828
Cl2	-30.001476	0.000279	0.085654	0.000374	0.094000	-5.236972	0.234638
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
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
CS	-15.817846	0.000198	0.265623	0.000204	0.274000	-5.256451	0.128007
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
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
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
H3CSH	-18.292741	0.000585	0.740583	0.000593	0.757000	-10.301775	0.372099
HCl	-15.626549	0.000119	0.168654	0.000174	0.171000	-1.472062	0.108954
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
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
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
NaCl							
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

(b) MAD = 5.40 +/- 0.16

(c) Figure



3.2 pVTZ, BFD

BeH removed because of pseudopotential instabilities in QMC

3.2.1 CCSD(T)/cc-pVTZ : 8.09

3.2.2 TODO CCSD(T)/VTZ-BFD :

3.2.3 PBE0/VTZ-BFD : 6.44

3.2.4 TODO $\mu = 0$

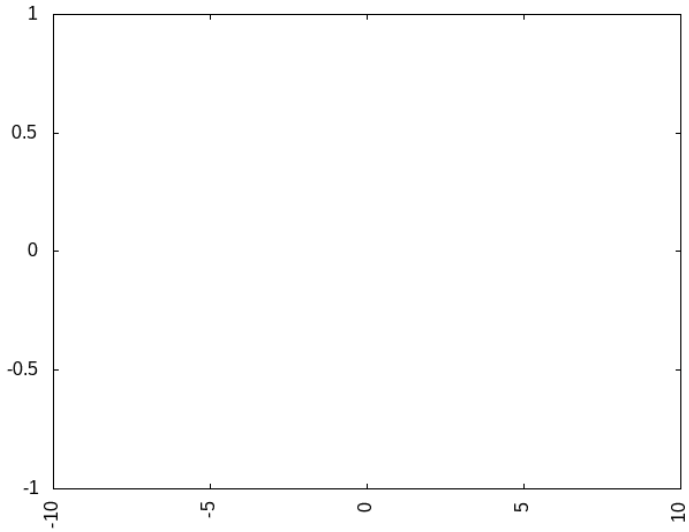
1. CIPSI

   (a) Table

e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
		MAD	

   (b) MAD =

   (c) Figure



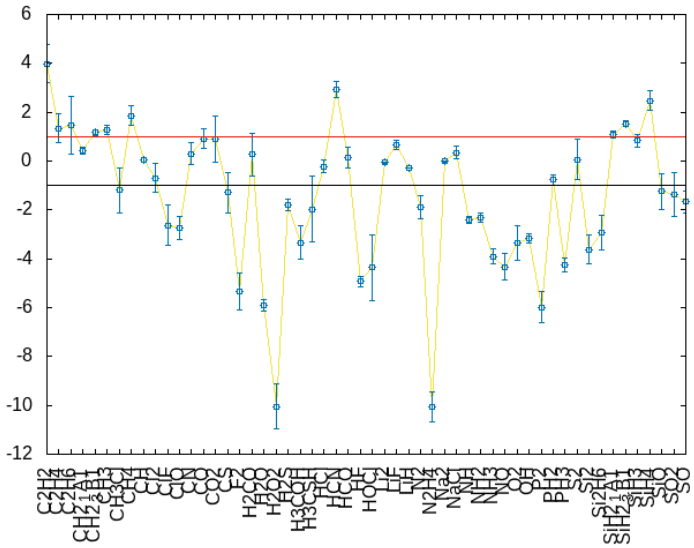
2. **TODO** QMC with Jastrow

   (a) Table

Total E Hartree	Delta E Hartree	Reference Hartree	Error kcal/mol	
			2.49	0.17

   (b) MAD =

   (c) Figure



3.2.5 DONE $\mu = 1/4$

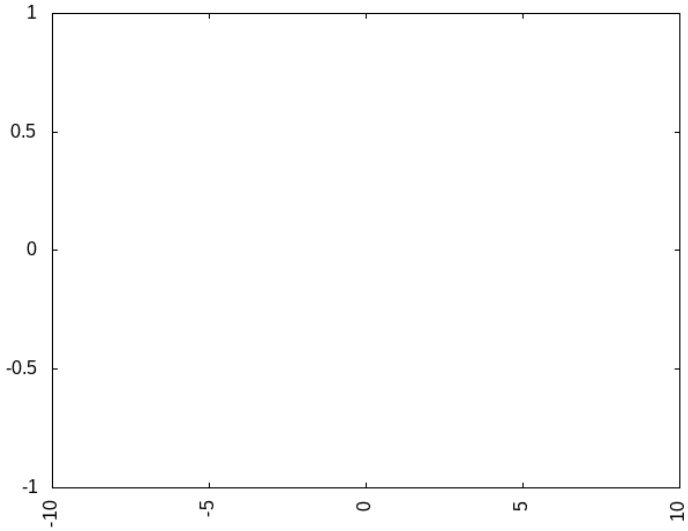
1. CIPSI

   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.994638			
C	-5.418798			
Cl	-14.939612			
F	-24.191803			
H	-0.498892			
Li	-0.198879			
N	-9.787920			
Na	-0.184562			
O	-15.896821			
P	-6.462610			
S	-10.108434			
Si	-3.760535			
BeH	-1.580067	0.086537	0.079400	4.478799
C2H2	-12.488247	0.652867	0.642400	6.568077
C2H4	-13.737941	0.904777	0.899000	3.625083
C2H6	-14.971590	1.140641	1.136900	2.347662
$CH2_{1A1}$	-6.698159	0.281577	0.288900	-4.595339
$CH2_{3B1}$	-6.723904	0.307321	0.304100	2.021468
CH3	-7.407165	0.491690	0.490800	0.558782
CH3Cl	-22.488919	0.633833	0.631000	1.777928
CH4	-8.082097	0.667731	0.670300	-1.612386
CH	-6.049247	0.131557	0.133900	-1.470090
Cl2	-29.982036	0.102812	0.094000	5.529465
ClF	-39.243721	0.112307	0.100100	7.659794
ClO	-30.955604	0.119172	0.104700	9.081158
CN	-15.500503	0.293785	0.288800	3.128016
CO	-21.736860	0.421241	0.413700	4.731779
CO2	-37.860561	0.648121	0.621400	16.767976
CS	-15.801669	0.274437	0.274000	0.274226
F2	-48.459597	0.075991	0.062200	8.654136
H2CO	-22.920253	0.606850	0.596700	6.369094
H2O	-17.255917	0.361313	0.371900	-6.643652
H2O2	-33.221051	0.429625	0.429400	0.141428
H2S	-11.392667	0.286450	0.292000	-3.482939
H3COH	-24.132017	0.820830	0.818700	1.336494
H3CSH	-18.278197	0.755397	0.757000	-1.005804
HCl	-15.606246	0.167743	0.171000	-2.044105
HCN	-16.212193	0.506583	0.496900	6.076107
HCO	-22.272113	0.457603	0.444700	8.096455
HF	-24.907592	0.216897	0.226100	-5.775072
HOCl	-31.605676	0.270351	0.264700	3.546025
Li2	-0.427789	0.030031	0.038900	-5.565398
LiF	-24.612130	0.221448	0.222000	-0.346485
LiH	-0.785226	0.087455	0.092430	-3.122037
N2	-19.946137	0.370297	0.364600	3.574839
N2H4	-22.267523	0.696115	0.699600	-2.186674
Na2	-0.390144	0.021020	0.026800	-3.627266

(b) MAD = 4.58

(c) Figure



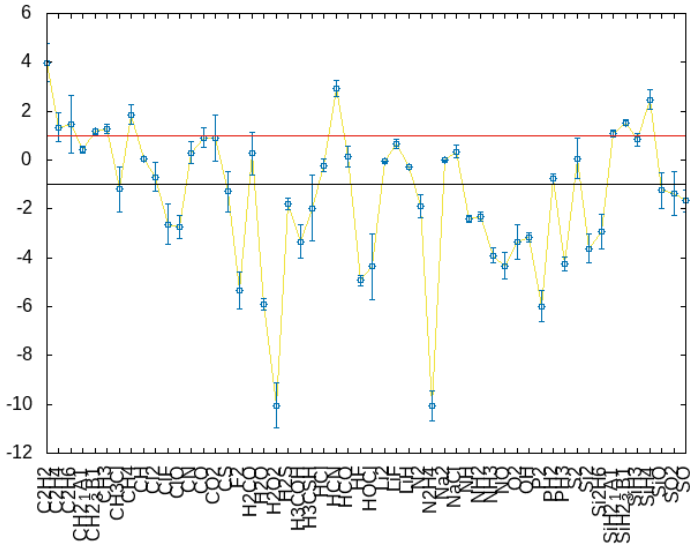
2. QMC with Jastrow

   (a) Table

	Total E Hartree		Delta E Hartree		Reference Hartree	Error kcal/mol	
Be	-1.001590	0.000043	0.000000	0.000061		0.000000	0.037971
C	-5.417927	0.000054	0.000000	0.000077		0.000000	0.048005
Cl	-14.944713	0.000094	0.000000	0.000132		0.000000	0.083062
F	-24.189771	0.000124	0.000000	0.000175		0.000000	0.109671
H	-0.500003	0.000003	0.000000	0.000005		0.000000	0.002880
Li	-0.196326	0.000001	0.000000	0.000002		0.000000	0.001228
N	-9.789147	0.000096	0.000000	0.000136		0.000000	0.085566
Na	-0.182144	0.000002	0.000000	0.000002		0.000000	0.001489
O	-15.892839	0.000100	0.000000	0.000141		0.000000	0.088594
P	-6.464868	0.000110	0.000000	0.000155		0.000000	0.097465
S	-10.111848	0.000104	0.000000	0.000147		0.000000	0.091983
Si	-3.760170	0.000093	0.000000	0.000131		0.000000	0.082432
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
$CH2_{1A1}$	-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
CH4	-8.094889	0.000260	0.676949	0.000266	0.670300	4.172378	0.166671
CH	-6.051869	0.000149	0.133939	0.000158	0.133900	0.024473	0.099450
Cl2	-29.983444	0.000262	0.094019	0.000322	0.094000	0.011860	0.202027
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
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
CS	-15.801754	0.000473	0.271980	0.000487	0.274000	-1.267778	0.305696
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
H3CSH	-18.292972	0.003027	0.763185	0.003029	0.757000	3.881053	1.900931
HCl	-15.614199	0.000231	0.169483	0.000249	0.171000	-0.951770	0.156484
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
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
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
Na2	-0.390920	0.000014	0.026633	0.000015	0.026800	-0.104782	0.009254

(b) MAD = 2.87 +/- 0.71

(c) Figure



3.2.6 DONE $\mu = 1/2$

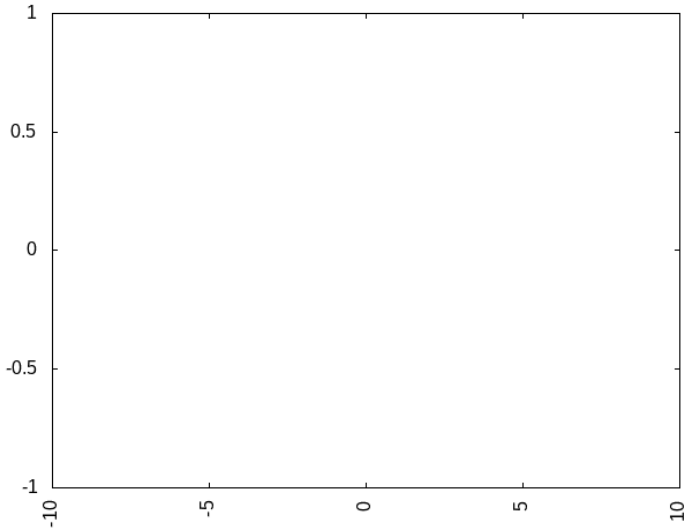
1. CIPSI

   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.998262			
C	-5.426287			
Cl	-14.945871			
F	-24.216187			
H	-0.502296			
Li	-0.196739			
N	-9.802906			
Na	-0.182371			
O	-15.914975			
P	-6.465047			
S	-10.111838			
Si	-3.759602			
C2H2	-12.491868	0.634701	0.642400	-4.831432
C2H4	-13.744979	0.883220	0.899000	-9.902176
C2H6	-14.984867	1.118515	1.136900	-11.536821
$CH2_{1A1}$	-6.704228	0.273349	0.288900	-9.758615
$CH2_{3B1}$	-6.732656	0.301776	0.304100	-1.458423
CH3	-7.415705	0.482530	0.490800	-5.189750
CH3Cl	-22.496886	0.617839	0.631000	-8.258935
CH4	-8.091636	0.656164	0.670300	-8.870454
CH	-6.054906	0.126323	0.133900	-4.754955
Cl2	-29.984427	0.092684	0.094000	-0.825724
ClF	-39.259993	0.097935	0.100100	-1.358376
ClO	-30.961899	0.101053	0.104700	-2.288617
CN	-15.500623	0.271430	0.288800	-10.899857
CO	-21.746748	0.405486	0.413700	-5.154533
CO2	-37.874991	0.618753	0.621400	-1.660920
CS	-15.799741	0.261616	0.274000	-7.771368
F2	-48.486273	0.053899	0.062200	-5.208688
H2CO	-22.931847	0.585993	0.596700	-6.719052
H2O	-17.271322	0.351755	0.371900	-12.641249
H2O2	-33.239150	0.404607	0.429400	-15.557645
H2S	-11.395645	0.279215	0.292000	-8.022687
H3COH	-24.150723	0.800276	0.818700	-11.561197
H3CSH	-18.285085	0.737775	0.757000	-12.063768
HCl	-15.611645	0.163478	0.171000	-4.720164
HCN	-16.216291	0.484802	0.496900	-7.591671
HCO	-22.281172	0.437613	0.444700	-4.447041
HF	-24.930165	0.211682	0.226100	-9.047528
HOCl	-31.616075	0.252932	0.264700	-7.384381
Li2	-0.429005	0.035528	0.038900	-2.116218
LiF	-24.633580	0.220654	0.222000	-0.844350
LiH	-0.785530	0.086495	0.092430	-3.724376
N2	-19.952279	0.346468	0.364600	-11.377891
N2H4	-22.281405	0.666410	0.699600	-20.827273
Na2	-0.389555	0.024814	0.026800	-1.246371
NaCl	-15.283496	0.155254	0.157400	-1.346838

(b) MAD = 6.87

(c) Figure



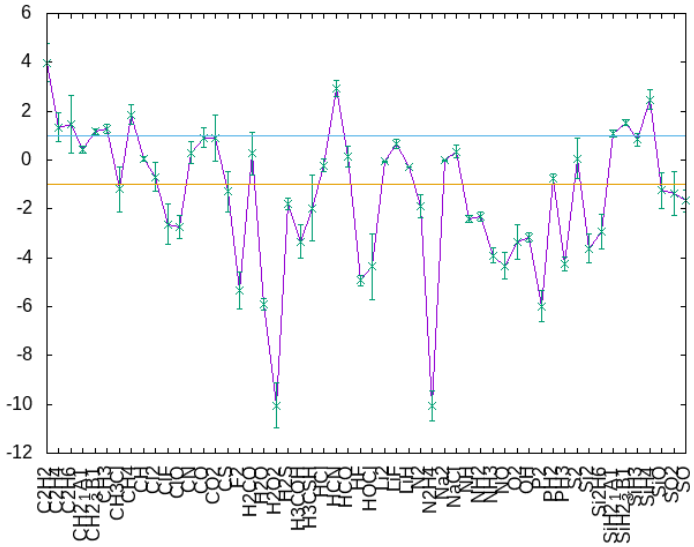
2. QMC without Jastrow

   (a) Table

	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
$CH2_{1A1}$	-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
CH	-6.056925	0.000143	0.133954	0.000155	0.133900	0.033677	0.097047
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
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
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
HCl	-15.623938	0.000347	0.170638	0.000405	0.171000	-0.226874	0.254259
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
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
Na2	-0.391055	0.000005	0.026768	0.000006	0.026800	-0.020205	0.003912
NaCl	-15.293398	0.000342	0.157958	0.000401	0.157400	0.349899	0.251619

(b) MAD = 2.30 +/- 0.60

(c) Figure



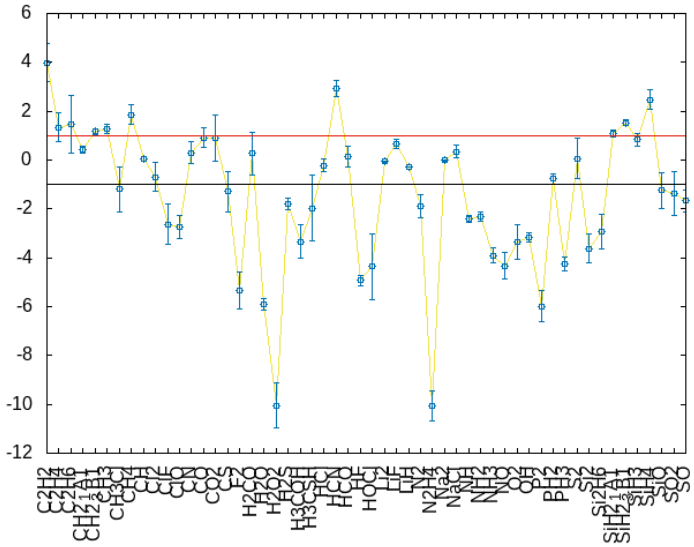
3. QMC with Jastrow

(a) Table

	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					
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
$CH2_{1A1}$	-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
CH4	-8.094962	0.000117	0.671721	0.000128	0.670300	0.891799	0.080400
CH	-6.057005	0.000034	0.133720	0.000045	0.133900	-0.113147	0.028276
Cl2	-29.998521	0.000254	0.093154	0.000283	0.094000	-0.530997	0.177333
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
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
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
H3CSH	-18.294959	0.000174	0.752693	0.000185	0.757000	-2.702788	0.116026
HCl	-15.622819	0.000098	0.170150	0.000117	0.171000	-0.533467	0.073175
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
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
Na2	-0.391058	0.000020	0.026784	0.000024	0.026800	-0.010004	0.015159
NaCl	-15.292371	0.000103	0.157551	0.000121	0.157400	0.094553	0.075647

(b) MAD = 2.49 +/- 0.17

(c) Figure



3.2.7 TODO $\mu = 1$

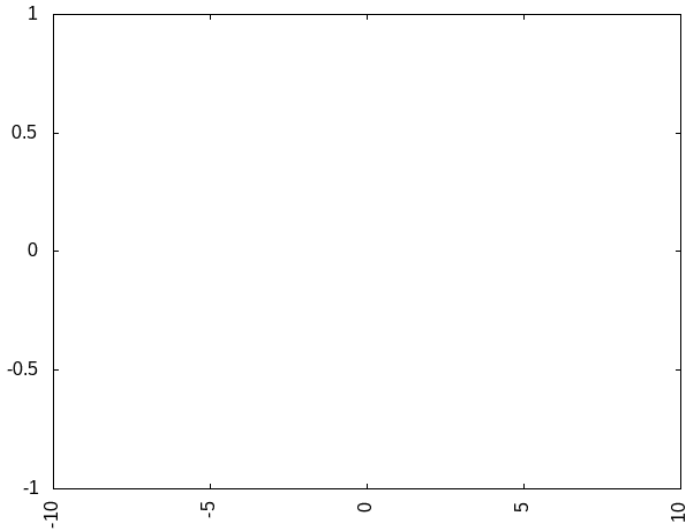
1. CIPSI

   (a) Table

e_{cal}	ae_{cal}	ae_{nr}	ae_{diff}
Hartree	Hartree	Hartree	kcal/mol
		MAD	

   (b) MAD =

   (c) Figure



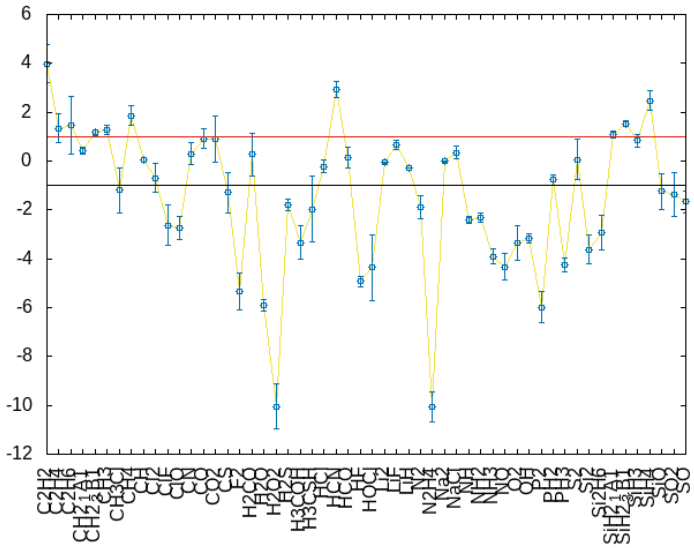
2. **TODO** QMC with Jastrow

   (a) Table

Total E Hartree	Delta E Hartree	Reference Hartree	Error kcal/mol	
			2.49	0.17

   (b) MAD =

   (c) Figure



3.3 pVQZ, BFD

3.3.1 CCSD(T)/cc-pVTZ : 7.99

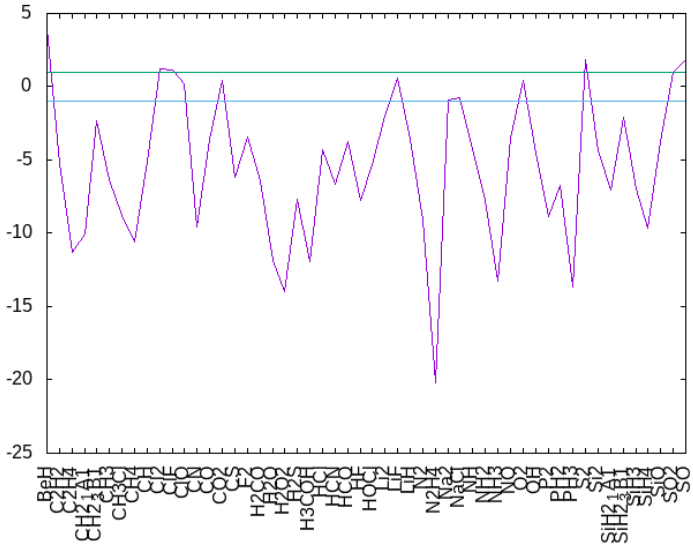
3.3.2 TODO $\mu = 1/2$

1. **DONE** CIPSI
   (a) Table

	e_{cal} Hartree	ae_{cal} Hartree	ae_{nr} Hartree	ae_{diff} kcal/mol
Be	-0.999244			
C	-5.426998			
Cl	-14.947964			
F	-24.217393			
H	-0.503289			
Li	-0.196938			
N	-9.803449			
Na	-0.182546			
O	-15.916012			
P	-6.465937			
S	-10.113623			
Si	-3.760405			
BeH	-1.588237	0.085704	0.079400	3.955757
C2H2	-12.494691	0.634115	0.642400	-5.198991
C2H4	-13.748208	0.881053	0.899000	-11.261902
$CH2_{1A1}$	-6.706420	0.272842	0.288900	-10.076400
$CH2_{3B1}$	-6.733935	0.300358	0.304100	-2.348100
CH3	-7.417628	0.480761	0.490800	-6.299356
CH3Cl	-22.501861	0.617031	0.631000	-8.765633
CH4	-8.093577	0.653421	0.670300	-10.591717
CH	-6.056113	0.125825	0.133900	-5.067187
Cl2	-29.991909	0.095982	0.094000	1.243454
ClF	-39.267335	0.101978	0.100100	1.178535
ClO	-30.969026	0.105051	0.104700	0.220009
CN	-15.503961	0.273514	0.288800	-9.592282
CO	-21.750950	0.407940	0.413700	-3.614443
CO2	-37.881120	0.622099	0.621400	0.438449
CS	-15.804719	0.264098	0.274000	-6.213870
F2	-48.491509	0.056722	0.062200	-3.437436
H2CO	-22.936125	0.586536	0.596700	-6.378001
H2O	-17.275666	0.353076	0.371900	-11.812535
H2O2	-33.245714	0.407112	0.429400	-13.985917
H2S	-11.399974	0.279772	0.292000	-7.673428
H3COH	-24.155854	0.799686	0.818700	-11.931540
HCl	-15.615378	0.164125	0.171000	-4.314148
HCN	-16.220032	0.486295	0.496900	-6.654462
HCO	-22.285095	0.438795	0.444700	-3.705432
HF	-24.934444	0.213761	0.226100	-7.742622
HOCl	-31.623491	0.256226	0.264700	-5.317269
Li2	-0.429619	0.035744	0.038900	-1.980329
LiF	-24.637272	0.222941	0.222000	0.590569
LiH	-0.786895	0.086668	0.092430	-3.615549
N2	-19.957050	0.350153	0.364600	-9.065931
N2H4	-22.287467	0.667412	0.699600	-20.198424
Na2	-0.390409	0.025317	0.026800	-0.930611
NaCl	-15.286774	0.156265	0.157400	-0.712297
NH	-10.433384	0.126646	0.133500	-4.300974

(b) MAD = 5.92

(c) Figure



2. **TODO** QMC

3.3.3 TODO $\mu = 1/4$

3.3.4 TODO $\mu = 0$

3.4 cc-pVDZ, ccECP

Variance is much higher than BFD

3.4.1 ExFCI : 16.75

3.4.2 $\mu = 1/2$

1. CIPSI 8.70
2. **TODO** QMC

3.4.3 Variances

	ccECP			BFD	
BeH	0.2569732117	0.0014377574	BeH	0.1782559715	0.0003249500
Be	0.1666086516	0.0016317663	Be	0.0350081316	0.0000455189
C2H2	5.6374376780	0.0647961759	C2H2	1.7700199505	0.0047449764
C2H4	5.8712017976	0.4533427056	C2H4	2.0967280411	0.2441935689
C2H6	5.7771151479	0.0935366539	C2H6	2.2770386967	0.0067776742
CH2	2.9382994304	0.0768249378	CH2	0.8563828486	0.0080716776
CH2	2.7514920039	0.0249987287	CH2	0.7864617103	0.0014011183
CH3Cl	7.6238640700	0.3160538174	CH3Cl	2.3222359454	0.0117067068
CH3	2.9613790384	0.0308869077	CH3	1.0499600172	0.0025989978
CH4	2.8991746692	0.0167518311	CH4	1.2534410879	0.0040565147
CH	2.8801149642	0.0285026971	CH	0.6323615876	0.0011958937
Cl2	9.2049628430	0.4329592940	Cl2	2.4689803260	0.0087148877
ClF	18.6535852385	1.0841356806	ClF	5.4733766010	0.0358697116
ClO	15.9917320532	0.4743905805	ClO	3.7455954039	0.0084052310
Cl	4.5107972815	0.0365469076	Cl	1.1109637114	0.0037441806
CN	6.3111506488	0.0286421038	CN	2.0384157705	0.0044778941
CO2	21.4168484794	0.1470078810	CO2	6.3465782442	0.0750875586
CO	12.6347545348	0.0840792838	CO	3.3332179742	0.0071374092
CS	5.6933223878	0.2229620761	CS	1.4313845164	0.0056034526
C	2.7555326925	0.0096528040	C	0.3948178125	0.0009312017
F2	27.8666039896	0.5862432312	F2	8.2505965114	0.0192749216
F	13.6157344746	0.0453868884	F	3.9077021624	0.0047515334
H2CO	13.4807720034	0.2507098917	H2CO	3.6466520145	0.0280906454
H2O2	19.2386065517	0.1290106584	H2O2	5.4717402756	0.0738831956
H2O	9.7734909194	0.0353955787	H2O	2.9039147949	0.0054009093
H2S	3.0445731672	0.0485033539	H2S	1.0177425450	0.0024233065
H3COH	12.0681704483	0.1983655994	H3COH	3.9032777719	0.0194556334
H3CSH	5.4593196842	0.0710795428	H3CSH	2.0602091587	0.0140420808
HCl	4.7318773631	0.0884534156	HCl	1.3336930551	0.0026891159
HCN	6.5324400169	0.0584962800	HCN	2.3210157020	0.0098303503
HCO	12.4795992761	0.1184051534	HCO	3.4014956049	0.0098780909
HF	13.6336168635	0.0273235443	HF	4.4447993272	0.0079686832
HOCl	21.0465588508	1.6546056962	HOCl	3.9399144603	0.0145241639
H	0.0096926772	0.0000006172	H	0.0018478787	0.0000001347
Li2	0.0413567058	0.0004204714	Li2	0.0071372698	0.0000155161
LiF	13.5336669006	0.0255991041	LiF	4.3113153968	0.0266129308
LiH	0.1161042913	0.0001613931	LiH	0.0992891351	0.0001972801
Li	0.0094982044	0.0002155035	Li	0.0009435223	0.0000002927
N2H4	7.5852332651	0.0529960389	N2H4	3.5022325222	0.0135003142
N2	7.5250942865	0.0395462903	N2	2.9100688888	0.0095335221
Na2	0.0546317711	0.0022970924	Na2	0.0125078559	0.0000213580
NaCl	4.6523587646	0.0884632260	NaCl	1.2823081139	0.0067196923
Na	0.0137537466	0.0004807667	Na	0.0042856342	0.0000018034
NH2	3.7938684003	0.0181874273	NH2	1.5805687564	0.0038447556
NH3	3.9666907409	0.1133016792	NH3	1.8904140849	0.0047380156
NH	3.6142835108	0.0092950350	NH	1.2365229242	0.0017477589
NO	13.3463483957	0.0873193711	NO	3.9621992615	0.0281738278
N	3.4081117947	0.0069017398	N	0.8636289136	0.0015720660

3.5 cc-pVTZ, ccECP

3.5.1 ExFCI : 4.73

3.5.2 $\mu = 1/2$

1. **TODO** CIPSI : RUNNING
2. **TODO** QMC

4 RUNNING

- TODO : mu=1 TZ CIPSI C2H6, Si2H6, H3CSH
- QZ 342441 rome Si2.sub scemama R 3:26 1 irene4046

5 TODO More calculations [0/10]

- ☐ ECMD des differents calculs RS-CIPSI
- ☐ DMC DZ FCI
- ☐ DMC DZ Hartree-Fock
- ☐ DMC TZ FCI (tres cher...)
- ☐ DMC TZ mu=1.e-6
- ☐ DMC TZ Hartree-Fock