Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Real Space bond orders are energetic descriptors
Electronic Suppementary Information.

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Contents

1 Raw data for Figure 1

Figure 1 is constructed from two data sets. In the first one, all calculations have been performed at the RHF//6-311G(d,p) level with GAMESS-US [1]. Geometries, as well as distances, covalent and ionic bond orders, and approximate and exact covalent and electrostatic energies for each pair of interactions in atomic units.

The second data set contains interaction energies for the following set of molecules, obtained at the CCSD(T)/aug-cc-pvdz level. Geometries have been taken from the NIST, KB49 or S22 data bases [2, 3, 4, 5], or optimized at the CCSD/aug-cc-pvdz level with GAMESS-US [1]. Density matrices where obtained with the pySCF suite [6]. IQA calculations where performed with promolden [7].

Molecule	Geometry
HNC	NIST
FCN	NIST
HF···CO	optimized
HCN···HF	KB49
CH_4	NIST
H_2CF^+	optimized
HCN	NIST
C_2H_4	NIST
HF···HF	KB49
H_2O	optimized
CH_4···HF	KB49
CH_4···CH_4	S22
H_2O···H_2O	optimized
OC···BH_3	optimized
CH_4···NH_3	KB49
HF···N_2	optimized
H_2CO···H_2CO	optimized
HCOOH	NIST
HF···H_2O	optimized
HF···F_2	optimized
NH_3···F_2	optimized
CH_3F···CH_3F	KB49
NH_3···NH_3	S22
H_2CO	NIST
HF···ClF	optimized
NH_3	NIST
BH_3	NIST
CH_3OH	NIST
C_2H_2	NIST
NO···NO	NIST

RHF DATA:

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======================================================================

 # File: bh3-nh3b.wfn
 # Number of Centers:   8
 # Molecule:H (  6)B (  1)N (  1)
 # Molecular Weight:     30.864100
 # Cartesian coordinates of centers:

        1   B      0.00000000    0.00000000    1.66488686
        2   N      0.00000000    0.00000000   -1.57290411
        3   H     -1.10435302    1.91279554    2.24198341
        4   H     -1.10435302   -1.91279554    2.24198341
        5   H      2.20870603    0.00000000    2.24198341
        6   H     -0.88416491    1.53141854   -2.24868396
        7   H     -0.88416491   -1.53141854   -2.24868396
        8   H      1.76832981    0.00000000   -2.24868396

 # Number of Primitives         :  126    reduced to  126
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
----------------------------------------------------------------------------------------------------
 1  2     3.238     0.251     2.063    -1.170    -0.065667    -0.038761    -0.827217    -0.745259
 1  3     2.283     0.459     2.063    -0.718    -0.127478    -0.100603    -0.707567    -0.648633
 1  4     2.283     0.459     2.063    -0.718    -0.127478    -0.100603    -0.707567    -0.648633
 1  5     2.283     0.459     2.063    -0.718    -0.127478    -0.100603    -0.707567    -0.648633
 1  6     4.295     0.004     2.063     0.422    -0.000433    -0.000458     0.218479     0.202536
 1  7     4.295     0.004     2.063     0.422    -0.000433    -0.000458     0.218479     0.202536
 1  8     4.295     0.004     2.063     0.422    -0.000433    -0.000458     0.218479     0.202536
 2  3     4.408     0.131    -1.170    -0.718    -0.024851    -0.014805     0.211776     0.190492
 2  4     4.408     0.131    -1.170    -0.718    -0.024851    -0.014805     0.211776     0.190492
 2  5     4.408     0.131    -1.170    -0.718    -0.024851    -0.014805     0.211776     0.190492
 2  6     1.893     0.813    -1.170     0.422    -0.251063    -0.214807    -0.196817    -0.260561
 2  7     1.893     0.813    -1.170     0.422    -0.251063    -0.214807    -0.196817    -0.260561
 2  8     1.893     0.813    -1.170     0.422    -0.251063    -0.214807    -0.196817    -0.260561
 3  4     3.826     0.148    -0.718    -0.718    -0.025667    -0.019383     0.152228     0.134696
 3  5     3.826     0.148    -0.718    -0.718    -0.025667    -0.019383     0.152228     0.134696
 3  6     4.512     0.007    -0.718     0.422    -0.000972    -0.000750    -0.071942    -0.067082
 3  7     5.664     0.003    -0.718     0.422    -0.000261    -0.000296    -0.059277    -0.053444
 3  8     5.664     0.003    -0.718     0.422    -0.000261    -0.000296    -0.059277    -0.053444
 6  7     3.063     0.013     0.422     0.422    -0.001570    -0.002055     0.071783     0.058051
 6  8     3.063     0.013     0.422     0.422    -0.001570    -0.002055     0.071783     0.058051
======================================================================

 # File: bh3-nh3.wfn
 # Number of Centers:   8
 # Molecule:H (  6)B (  1)N (  1)
 # Molecular Weight:     30.864100
 # Cartesian coordinates of centers:

        1   B      0.00000000    0.00000000    1.62351857
        2   N      0.00000000    0.00000000   -1.55163746
        3   H     -1.10635500    1.91626307    2.19991746
        4   H     -1.10635500   -1.91626307    2.19991746
        5   H      2.21271000    0.00000000    2.19991746
        6   H     -1.77104102    0.00000000   -2.22387783
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       7   H      0.88552051   -1.53376651   -2.22387783
       8   H      0.88552051    1.53376651   -2.22387783

 # Number of Primitives         :  126    reduced to  126
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     3.175     0.259     2.068    -1.172    -0.069134    -0.040855    -0.855157    -0.763158
 1  3     2.287     0.455     2.068    -0.715    -0.126264    -0.099487    -0.703724    -0.646775
 1  4     2.287     0.455     2.068    -0.715    -0.126264    -0.099487    -0.703724    -0.646775
 1  5     2.287     0.455     2.068    -0.715    -0.126264    -0.099487    -0.703724    -0.646775
 1  6     4.235     0.004     2.068     0.419    -0.000456    -0.000473     0.221410     0.204628
 1  7     4.235     0.004     2.068     0.419    -0.000456    -0.000473     0.221410     0.204628
 1  8     4.235     0.004     2.068     0.419    -0.000456    -0.000473     0.221410     0.204628
 2  3     4.355     0.138    -1.172    -0.715    -0.026495    -0.015805     0.214565     0.192479
 2  4     4.355     0.138    -1.172    -0.715    -0.026495    -0.015805     0.214565     0.192479
 2  5     4.355     0.138    -1.172    -0.715    -0.026495    -0.015805     0.214565     0.192479
 2  6     1.894     0.813    -1.172     0.419    -0.251146    -0.214619    -0.196106    -0.259355
 2  7     1.894     0.813    -1.172     0.419    -0.251146    -0.214619    -0.196106    -0.259355
 2  8     1.894     0.813    -1.172     0.419    -0.251146    -0.214619    -0.196106    -0.259355
 3  4     3.833     0.146    -0.715    -0.715    -0.025201    -0.019002     0.150549     0.133502
 3  5     3.833     0.146    -0.715    -0.715    -0.025201    -0.019002     0.150549     0.133502
 3  6     4.867     0.003    -0.715     0.419    -0.000401    -0.000324    -0.067218    -0.061614
 3  7     5.953     0.008    -0.715     0.419    -0.000615    -0.000698    -0.056186    -0.050368
 3  8     4.867     0.003    -0.715     0.419    -0.000401    -0.000324    -0.067218    -0.061614
 6  7     3.068     0.013     0.419     0.419    -0.001568    -0.002058     0.071033     0.057286
 6  8     3.068     0.013     0.419     0.419    -0.001568    -0.002058     0.071033     0.057286
=================================================================

 # File: butane.wfn
 # Number of Centers:  14
 # Molecule:H ( 10)C (  4)
 # Molecular Weight:     58.122999
 # Cartesian coordinates of centers:

       1   C      3.42754215    1.39299779    0.00000000
       2   C     -3.42754215   -1.39299779    0.00000000
       3   C      0.54247704    1.33802217    0.00000000
       4   C     -0.54247704   -1.33802217    0.00000000
       5   H      4.13287608    3.31755641    0.00000000
       6   H     -4.13287608   -3.31755641    0.00000000
       7   H      4.18457870    0.44930305    1.65673702
       8   H     -4.18457870   -0.44930305   -1.65673702
       9   H      4.18457870    0.44930305   -1.65673702
      10   H     -4.18457870   -0.44930305    1.65673702
      11   H     -0.15818719    2.35133169    1.64449696
      12   H      0.15818719   -2.35133169   -1.64449696
      13   H     -0.15818719    2.35133169   -1.64449696
      14   H      0.15818719   -2.35133169    1.64449696

 # Number of Primitives         :  246    reduced to  242
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     7.400     0.009     0.161     0.161    -0.000739    -0.000641     0.003429     0.003495
 1  3     2.886     0.980     0.161     0.163    -0.299847    -0.169815     0.028172     0.009062
 1  4     4.819     0.044     0.161     0.163    -0.006906    -0.004569     0.006029     0.005426
 1  5     2.050     0.967     0.161    -0.057    -0.285864    -0.235776     0.031294    -0.004452
 1  6     8.908     0.002     0.161    -0.057    -0.000103    -0.000109    -0.000766    -0.001024
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1	7	2.051	0.964	0.161	-0.060	-0.285161	-0.234837	0.030742	-0.004716
1	8	8.005	0.001	0.161	-0.060	-0.000051	-0.000046	-0.001044	-0.001208
1	9	2.051	0.964	0.161	-0.060	-0.285161	-0.234837	0.030742	-0.004716
1	10	8.005	0.001	0.161	-0.060	-0.000051	-0.000046	-0.001044	-0.001208
1	11	4.060	0.043	0.161	-0.073	-0.006568	-0.005344	-0.001041	-0.002887
1	12	5.236	0.007	0.161	-0.073	-0.001059	-0.000714	-0.001804	-0.002239
1	13	4.060	0.043	0.161	-0.073	-0.006568	-0.005344	-0.001041	-0.002887
1	14	5.236	0.007	0.161	-0.073	-0.001059	-0.000714	-0.001804	-0.002239
3	4	2.888	0.968	0.163	0.163	-0.298764	-0.167554	0.026666	0.009156
3	5	4.100	0.042	0.163	-0.057	-0.006030	-0.005062	-0.000422	-0.002250
3	6	6.598	0.010	0.163	-0.057	-0.000786	-0.000785	-0.000851	-0.001398
3	7	4.099	0.041	0.163	-0.060	-0.005886	-0.005018	-0.000442	-0.002387
3	8	5.318	0.007	0.163	-0.060	-0.000885	-0.000624	-0.001450	-0.001839
3	9	4.099	0.041	0.163	-0.060	-0.005886	-0.005018	-0.000442	-0.002387
3	10	5.318	0.007	0.163	-0.060	-0.000885	-0.000624	-0.001450	-0.001839
3	11	2.055	0.949	0.163	-0.073	-0.283427	-0.230808	0.027714	-0.005768
3	12	4.058	0.042	0.163	-0.073	-0.006256	-0.005138	-0.001042	-0.002921
3	13	2.055	0.949	0.163	-0.073	-0.283427	-0.230808	0.027714	-0.005768
3	14	4.058	0.042	0.163	-0.073	-0.006256	-0.005138	-0.001042	-0.002921
5	6	10.599	0.000	-0.057	-0.057	-0.000021	-0.000023	0.000200	0.000304
5	7	3.313	0.043	-0.057	-0.060	-0.006233	-0.006554	0.001312	0.001030
5	8	9.280	0.000	-0.057	-0.060	-0.000003	-0.000003	0.000298	0.000368
5	9	3.313	0.043	-0.057	-0.060	-0.006233	-0.006554	0.001312	0.001030
5	10	9.280	0.000	-0.057	-0.060	-0.000003	-0.000003	0.000298	0.000368
5	11	4.696	0.004	-0.057	-0.073	-0.000472	-0.000392	0.000812	0.000881
5	12	7.116	0.001	-0.057	-0.073	-0.000060	-0.000058	0.000359	0.000581
5	13	4.696	0.004	-0.057	-0.073	-0.000472	-0.000392	0.000812	0.000881
5	14	7.116	0.001	-0.057	-0.073	-0.000060	-0.000058	0.000359	0.000581
7	8	9.046	0.000	-0.060	-0.060	-0.000020	-0.000020	0.000270	0.000400
7	9	3.313	0.044	-0.060	-0.060	-0.006280	-0.006624	0.001347	0.001092
7	10	8.417	0.000	-0.060	-0.060	-0.000003	-0.000003	0.000376	0.000430
7	11	4.741	0.004	-0.060	-0.073	-0.000429	-0.000372	0.000804	0.000925
7	12	5.912	0.001	-0.060	-0.073	-0.000049	-0.000043	0.000559	0.000742
7	13	5.777	0.012	-0.060	-0.073	-0.000854	-0.001012	0.000392	0.000759
7	14	4.905	0.006	-0.060	-0.073	-0.001032	-0.000652	0.001081	0.000894
11	12	5.747	0.012	-0.073	-0.073	-0.000840	-0.001008	0.000504	0.000924
11	13	3.289	0.043	-0.073	-0.073	-0.006455	-0.006602	0.001591	0.001616
11	14	4.713	0.004	-0.073	-0.073	-0.000438	-0.000379	0.000957	0.001127

```
 # File: c2h2f2t.wfn
 # Number of Centers:   6
 # Molecule:H (  2)C (  2)F (  2)
 # Molecular Weight:     64.034606
 # Cartesian coordinates of centers:

        1   C     -1.23207653   -0.06510159    0.00000000
        2   C      1.23207653    0.06510159    0.00000000
        3   H     -2.31109261   -1.77828569    0.00000000
        4   H      2.31109261    1.77828569    0.00000000
        5   F     -2.60607988    2.02642489    0.00000000
        6   F      2.60607988   -2.02642489    0.00000000

 # Number of Primitives         :  160    reduced to  160
```

A	B	distance	delta	QA	QB	Vxc	Vxc(approx)	Vcl	Vcl(approx)
1	2	2.468	1.720	0.641	0.641	-0.514740	-0.348604	0.206402	0.166297

```
 1  3     2.025     0.931     0.641     0.078    -0.284471    -0.229869     0.069852     0.024650
 1  4     3.994     0.054     0.641     0.078    -0.006015    -0.006765    -0.432815     0.012496
 1  5     2.502     0.761     0.641    -0.718    -0.231906    -0.152039    -0.389625    -0.183854
 1  6     4.310     0.140     0.641    -0.718    -0.020019    -0.016279    -0.973843    -0.106743
 3  4     5.832     0.007     0.078     0.078    -0.000533    -0.000620     0.001863     0.001041
 3  5     3.816     0.061     0.078    -0.718    -0.009347    -0.008023    -0.023023    -0.014664
 3  6     4.923     0.011     0.078    -0.718    -0.001340    -0.001072    -0.050133    -0.011366
 5  6     6.602     0.022    -0.718    -0.718    -0.001753    -0.001631     0.086205     0.078131
=========================================================================

 # File: c2h2f2f.wfn
 # Number of Centers:   6
 # Molecule:H (  2)C (  2)F (  2)
 # Molecular Weight:     64.034606
 # Cartesian coordinates of centers:

        1   C     -1.23502175   -0.06589843    0.00000000
        2   C      1.23502175    0.06589843    0.00000000
        3   H     -2.32350148   -1.77135292    0.00000000
        4   H      2.32350148    1.77135292    0.00000000
        5   F     -2.58650290    2.02622395    0.00000000
        6   F      2.58650290   -2.02622395    0.00000000

 # Number of Primitives         :  160    reduced to  160
 A  B  distance      delta     QA     QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     2.474     1.715     0.645     0.645    -0.512408    -0.346639     0.206439     0.168078
 1  3     2.023     0.931     0.645     0.077    -0.284712    -0.230096     0.070080     0.024486
 1  4     4.005     0.054     0.645     0.077    -0.005986    -0.006743    -0.432358     0.012370
 1  5     2.491     0.762     0.645    -0.721    -0.233023    -0.152897    -0.395812    -0.186774
 1  6     4.295     0.143     0.645    -0.721    -0.020450    -0.016589    -0.976071    -0.108311
 3  4     5.843     0.007     0.077     0.077    -0.000524    -0.000610     0.001820     0.001010
 3  5     3.807     0.062     0.077    -0.721    -0.009461    -0.008110    -0.023013    -0.014562
 3  6     4.917     0.011     0.077    -0.721    -0.001346    -0.001078    -0.050064    -0.011274
 5  6     6.571     0.022    -0.721    -0.721    -0.001788    -0.001664     0.087353     0.079210
=========================================================================

 # File: c2h2f2c.wfn
 # Number of Centers:   6
 # Molecule:H (  2)C (  2)F (  2)
 # Molecular Weight:     64.034606
 # Cartesian coordinates of centers:

        1   C      0.00000000   -1.23502175    0.06589843
        2   C      0.00000000    1.23502175    0.06589843
        3   H      0.00000000   -2.32350148    1.77135292
        4   H      0.00000000    2.32350148    1.77135292
        5   F      0.00000000   -2.58650290   -2.02622395
        6   F      0.00000000    2.58650290   -2.02622395

 # Number of Primitives         :  160    reduced to  160
 A  B  distance      delta     QA     QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     2.470     1.723     0.648     0.648    -0.514866    -0.348726     0.223686     0.169815
 1  3     2.023     0.935     0.648     0.067    -0.285929    -0.231127     0.067721     0.021323
 1  4     3.946     0.059     0.648     0.067    -0.006963    -0.007437    -0.447892     0.010933
 1  5     2.491     0.762     0.648    -0.714    -0.233002    -0.152943    -0.396775    -0.185647
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 1  6     4.357     0.132     0.648    -0.714    -0.017694    -0.015098    -0.978179    -0.106132
 3  4     4.647     0.004     0.067     0.067    -0.000427    -0.000379     0.001695     0.000955
 3  5     3.807     0.062     0.067    -0.714    -0.009549    -0.008192    -0.021007    -0.012493
 3  6     6.207     0.012     0.067    -0.714    -0.000880    -0.000936    -0.039792    -0.007662
 5  6     5.173     0.030    -0.714    -0.714    -0.004365    -0.002902     0.105411     0.098535
=============================================================================

 # File: c2h6.wfn
 # Number of Centers:   8
 # Molecule:H (  6)C (  2)
 # Molecular Weight:     30.069399
 # Cartesian coordinates of centers:

        1   C      0.00000000    0.00000000   -1.44224916
        2   C      0.00000000    0.00000000    1.44224916
        3   H     -1.65547465   -0.95578874    2.18212032
        4   H      1.65547465   -0.95578874    2.18212032
        5   H      0.00000000   -1.91157747   -2.18212032
        6   H      1.65547465    0.95578874   -2.18212032
        7   H     -1.65547465    0.95578874   -2.18212032
        8   H      0.00000000    1.91157747    2.18212032

 # Number of Primitives         :  132    reduced to  130
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     2.884     0.994     0.171     0.171    -0.301154    -0.172347     0.030607     0.010079
 1  3     4.098     0.043     0.171    -0.057    -0.006194    -0.005257    -0.000392    -0.002372
 1  4     4.098     0.043     0.171    -0.057    -0.006194    -0.005257    -0.000392    -0.002372
 1  5     2.050     0.968     0.171    -0.057    -0.203028    -0.236022    -1.240950    -0.004742
 1  6     2.050     0.968     0.171    -0.057    -0.203028    -0.236022    -1.240950    -0.004742
 1  7     2.050     0.968     0.171    -0.057    -0.203028    -0.236022    -1.240950    -0.004742
 1  8     4.098     0.043     0.171    -0.057    -0.006194    -0.005257    -0.000392    -0.002372
 3  4     3.311     0.044    -0.057    -0.057    -0.006238    -0.006597     0.001297     0.000981
 3  5     4.765     0.003    -0.057    -0.057    -0.000419    -0.000366     0.000636     0.000682
 3  6     5.802     0.012    -0.057    -0.057    -0.000883    -0.001041     0.000277     0.000560
 3  7     4.765     0.003    -0.057    -0.057    -0.000419    -0.000366     0.000636     0.000682
 3  8     3.311     0.044    -0.057    -0.057    -0.006238    -0.006597     0.001297     0.000981
=============================================================================

 # File: ch2fohb.wfn
 # Number of Centers:   6
 # Molecule:H (  3)C (  1)O (  1)F (  1)
 # Molecular Weight:     50.032503
 # Cartesian coordinates of centers:

        1   C     -1.33804073    0.20291098    0.00000000
        2   O      1.25899557    0.12514464    0.00000000
        3   F     -2.26617379   -2.19496443    0.00000000
        4   H     -2.02025456    1.13190388   -1.68539213
        5   H     -2.02025456    1.13190388    1.68539213
        6   H      1.81922806   -1.56432809    0.00000000

 # Number of Primitives         :  144    reduced to  141
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     2.598     0.753     1.355    -1.282    -0.236301    -0.144844    -0.819268    -0.668552
 1  3     2.571     0.650     1.355    -0.734    -0.199864    -0.126491    -0.534845    -0.387118
```

```
 1  4     2.042     0.889     1.355     0.005    -0.277064    -0.217694     0.058760     0.003054
 1  5     2.042     0.889     1.355     0.005    -0.277064    -0.217694     0.058760     0.003054
 1  6     3.618     0.010     1.355     0.652    -0.001189    -0.001422     0.295113     0.244218
 2  3     4.220     0.165    -1.282    -0.734    -0.032021    -0.019506     0.243002     0.223014
 2  4     3.822     0.075    -1.282     0.005    -0.011760    -0.009806    -0.012016    -0.001542
 2  5     3.822     0.075    -1.282     0.005    -0.011760    -0.009806    -0.012016    -0.001542
 2  6     1.780     0.563    -1.282     0.652    -0.177830    -0.158172    -0.424812    -0.469400
 3  4     3.738     0.070    -0.734     0.005    -0.011579    -0.009420    -0.007993    -0.000904
 3  5     3.738     0.070    -0.734     0.005    -0.011579    -0.009420    -0.007993    -0.000904
 3  6     4.134     0.010    -0.734     0.652    -0.001730    -0.001262    -0.121136    -0.115818
 4  5     3.371     0.034     0.005     0.005    -0.004336    -0.004993     0.001527     0.000006
 4  6     4.985     0.002     0.005     0.652    -0.000179    -0.000224     0.003936     0.000602
=========================================================================


 # File: ch2fohf.wfn
 # Number of Centers:   6
 # Molecule:H (  3)C (  1)O (  1)F (  1)
 # Molecular Weight:     50.032503
 # Cartesian coordinates of centers:

        1   C     -1.37096030    0.19090201    0.00000000
        2   O      1.21702700   -0.07451568    0.00000000
        3   F     -2.34828123   -2.15135099    0.00000000
        4   H     -2.03543520    1.14785736    1.68571873
        5   H     -2.03543520    1.14785736   -1.68571873
        6   H      1.66655502   -1.79581417    0.00000000

 # Number of Primitives         :  144    reduced to  141
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.602     0.744     1.367    -1.285    -0.233481    -0.142942    -0.825422    -0.675198
 1  3     2.538     0.649     1.367    -0.742    -0.201709    -0.127836    -0.556253    -0.399609
 1  4     2.049     0.888     1.367     0.003    -0.276053    -0.216662     0.057524     0.002085
 1  5     2.049     0.888     1.367     0.003    -0.276053    -0.216662     0.057524     0.002085
 1  6     3.630     0.010     1.367     0.653    -0.001189    -0.001428     0.297597     0.246132
 2  3     4.126     0.178    -1.285    -0.742    -0.035863    -0.021515     0.249505     0.230994
 2  4     3.862     0.073    -1.285     0.003    -0.011277    -0.009466    -0.011296    -0.001040
 2  5     3.862     0.073    -1.285     0.003    -0.011277    -0.009466    -0.011296    -0.001040
 2  6     1.779     0.560    -1.285     0.653    -0.177174    -0.157388    -0.425951    -0.471905
 3  4     3.718     0.072    -0.742     0.003    -0.011906    -0.009667    -0.007989    -0.000623
 3  5     3.718     0.072    -0.742     0.003    -0.011906    -0.009667    -0.007989    -0.000623
 3  6     4.031     0.011    -0.742     0.653    -0.001977    -0.001423    -0.124906    -0.120262
 4  5     3.371     0.035     0.003     0.003    -0.004433    -0.005127     0.001490     0.000003
 4  6     5.021     0.002     0.003     0.653    -0.000178    -0.000222     0.003670     0.000407
=========================================================================


 # File: ch3beh.wfn
 # Number of Centers:   6
 # Molecule:H (  4)Be(  1)C (  1)
 # Molecular Weight:     25.054780
 # Cartesian coordinates of centers:

        1   H      0.00000000    0.00000000    5.60267531
        2   C      0.00000000    0.00000000   -0.12195953
        3   H     -0.95460565    1.65342549   -0.88899808
        4   H     -0.95460565   -1.65342549   -0.88899808
        5   H      1.90921130    0.00000000   -0.88899808
```

```
       6   BE     0.00000000    0.00000000    3.07600446

 # Number of Primitives         :  110    reduced to  108
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     5.725     0.095    -0.865    -0.738    -0.012424    -0.008304     0.173822     0.111546
 1  3     6.767     0.003    -0.865    -0.045    -0.000284    -0.000257     0.004159     0.005749
 1  4     6.767     0.003    -0.865    -0.045    -0.000284    -0.000257     0.004159     0.005749
 1  5     6.767     0.003    -0.865    -0.045    -0.000284    -0.000257     0.004159     0.005749
 1  6     2.527     0.260    -0.865     1.738    -0.060870    -0.051369    -0.628719    -0.595263
 2  3     2.058     1.036    -0.738    -0.045    -0.291502    -0.251675     0.036895     0.016126
 2  4     2.058     1.036    -0.738    -0.045    -0.291502    -0.251675     0.036895     0.016126
 2  5     2.058     1.036    -0.738    -0.045    -0.291502    -0.251675     0.036895     0.016126
 2  6     3.198     0.245    -0.738     1.738    -0.062668    -0.038276    -0.661174    -0.401125
 3  4     3.307     0.047    -0.045    -0.045    -0.006638    -0.007038     0.001294     0.000611
 3  5     3.307     0.047    -0.045    -0.045    -0.006638    -0.007038     0.001294     0.000611
 3  6     4.401     0.009    -0.045     1.738    -0.000939    -0.000979    -0.006542    -0.017759
=================================================================================

 # File: ch3bh2.wfn
 # Number of Centers:   7
 # Molecule:H (  5)B (  1)C (  1)
 # Molecular Weight:     27.860500
 # Cartesian coordinates of centers:

       1   C     -1.56929387    0.15315514    0.00000000
       2   B      1.39379487    0.05496759    0.00000000
       3   H     -2.19248349   -1.81875109    0.00000000
       4   H     -2.37483789    1.01661249   -1.67414670
       5   H     -2.37483789    1.01661249    1.67414670
       6   H      2.55115827   -0.03505223   -1.93148318
       7   H      2.55115827   -0.03505223    1.93148318

 # Number of Primitives         :  123    reduced to  121
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.965     0.468    -0.622     2.155    -0.138108    -0.078875    -0.823796    -0.452352
 1  3     2.068     1.003    -0.622    -0.025    -0.283946    -0.242461     0.031688     0.007578
 1  4     2.049     1.004    -0.622    -0.037    -0.290463    -0.245098     0.034132     0.011342
 1  5     2.049     1.004    -0.622    -0.037    -0.290463    -0.245098     0.034132     0.011342
 1  6     4.555     0.146    -0.622    -0.716    -0.026266    -0.016079     0.157875     0.097801
 1  7     4.555     0.146    -0.622    -0.716    -0.026266    -0.016079     0.157875     0.097801
 2  3     4.046     0.020     2.155    -0.025    -0.002557    -0.002526     0.001754    -0.013412
 2  4     4.234     0.013     2.155    -0.037    -0.001565    -0.001536    -0.003622    -0.019003
 2  5     4.234     0.013     2.155    -0.037    -0.001565    -0.001536    -0.003622    -0.019003
 2  6     2.253     0.476     2.155    -0.716    -0.133132    -0.105575    -0.776494    -0.684488
 2  7     2.253     0.476     2.155    -0.716    -0.133132    -0.105575    -0.776494    -0.684488
 3  4     3.298     0.043    -0.025    -0.037    -0.006354    -0.006567     0.001225     0.000285
 3  5     3.298     0.043    -0.025    -0.037    -0.006354    -0.006567     0.001225     0.000285
 3  6     5.423     0.007    -0.025    -0.716    -0.000776    -0.000675     0.001246     0.003323
 3  7     5.423     0.007    -0.025    -0.716    -0.000776    -0.000675     0.001246     0.003323
 4  5     3.348     0.043    -0.037    -0.037    -0.005850    -0.006354     0.001182     0.000416
 4  6     5.044     0.009    -0.037    -0.716    -0.001070    -0.000865     0.003445     0.005299
 4  7     6.195     0.011    -0.037    -0.716    -0.000655    -0.000887    -0.059985     0.004315
 6  7     3.863     0.146    -0.716    -0.716    -0.024919    -0.018856     0.159397     0.132627
=================================================================================
```

```
# File: ch3cf3.wfn
# Number of Centers:   8
# Molecule:H (  3)C (  2)F (  3)
# Molecular Weight:     84.040910
# Cartesian coordinates of centers:

       1   C      0.00000000    0.00000000   -0.17213588
       2   H     -0.96412665    1.66991634   -0.84455755
       3   H     -0.96412665   -1.66991634   -0.84455755
       4   H      1.92825329    0.00000000   -0.84455755
       5   C      0.00000000    0.00000000    2.66391155
       6   F      1.16005907   -2.00928126    3.59017315
       7   F      1.16005907    2.00928126    3.59017315
       8   F     -2.32011815    0.00000000    3.59017315

# Number of Primitives         :  222    reduced to  217
A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl          Vcl(approx)
-------------------------------------------------------------------------------------------------------
1  2     2.042     0.954     0.198     0.010    -0.284407    -0.233467     0.038742     0.000937
1  3     2.042     0.954     0.198     0.010    -0.284407    -0.233467     0.038742     0.000937
1  4     2.042     0.954     0.198     0.010    -0.284407    -0.233467     0.038742     0.000937
1  5     2.836     0.881     0.198     1.961    -0.288981    -0.155366     0.164293     0.137046
1  6     4.420     0.074     0.198    -0.730    -0.012783    -0.008410    -0.046046    -0.032735
1  7     4.420     0.074     0.198    -0.730    -0.012783    -0.008410    -0.046046    -0.032735
1  8     4.420     0.074     0.198    -0.730    -0.012783    -0.008410    -0.046046    -0.032735
2  3     3.340     0.035     0.010     0.010    -0.004954    -0.005291     0.001704     0.000028
2  4     3.340     0.035     0.010     0.010    -0.004954    -0.005291     0.001704     0.000028
2  5     4.003     0.040     0.010     1.961    -0.006398    -0.005053     0.012772     0.004728
2  6     6.141     0.012     0.010    -0.730    -0.000965    -0.000984    -0.003991    -0.001147
2  7     4.929     0.009     0.010    -0.730    -0.001224    -0.000918    -0.067216    -0.001430
2  8     4.929     0.009     0.010    -0.730    -0.001224    -0.000918    -0.067216    -0.001430
5  6     2.498     0.570     1.961    -0.730    -0.186244    -0.114124    -0.761976    -0.573167
5  7     2.498     0.570     1.961    -0.730    -0.186244    -0.114124    -0.761976    -0.573167
5  8     2.498     0.570     1.961    -0.730    -0.186244    -0.114124    -0.761976    -0.573167
6  7     4.019     0.167    -0.730    -0.730    -0.035624    -0.020761     0.156036     0.132651
6  8     4.019     0.167    -0.730    -0.730    -0.035624    -0.020761     0.156036     0.132651
=======================================================================

# File: ch3ch2f.wfn
# Number of Centers:   8
# Molecule:H (  5)C (  2)F (  1)
# Molecular Weight:     48.059903
# Cartesian coordinates of centers:

       1   C     -1.51603448   -0.21405237    0.00000000
       2   C      1.33828859   -0.24634020    0.00000000
       3   F      2.25087942    2.18370753    0.00000000
       4   H     -2.23051581   -2.13576293    0.00000000
       5   H     -2.22681929    0.74491337   -1.66273815
       6   H     -2.22681929    0.74491337    1.66273815
       7   H      2.08050265   -1.17413620   -1.66476007
       8   H      2.08050265   -1.17413620    1.66476007

# Number of Primitives         :  162    reduced to  159
A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl          Vcl(approx)
-------------------------------------------------------------------------------------------------------
1  2     2.855     0.963     0.163     0.717    -0.301015    -0.168756     0.061171     0.040877
```

```
 1  3     4.465     0.082     0.163    -0.732    -0.013953    -0.009147    -0.031202    -0.026687
 1  4     2.050     0.965     0.163    -0.040    -0.284924    -0.235253     0.033145    -0.003175
 1  5     2.047     0.962     0.163    -0.029    -0.285477    -0.235035     0.034415    -0.002294
 1  6     2.047     0.962     0.163    -0.029    -0.285477    -0.235035     0.034415    -0.002294
 1  7     4.078     0.038     0.163    -0.025    -0.005452    -0.004702     0.001174    -0.000978
 1  8     4.078     0.038     0.163    -0.025    -0.005452    -0.004702     0.001174    -0.000978
 2  3     2.596     0.707     0.717    -0.732    -0.212621    -0.136218    -0.359745    -0.202050
 2  4     4.038     0.044     0.717    -0.040    -0.006807    -0.005506    -0.001557    -0.007095
 2  5     4.057     0.042     0.717    -0.029    -0.006025    -0.005119    -0.000470    -0.005093
 2  6     4.057     0.042     0.717    -0.029    -0.006025    -0.005119    -0.000470    -0.005093
 2  7     2.045     0.924     0.717    -0.025    -0.282003    -0.225993     0.038311    -0.008585
 2  8     2.045     0.924     0.717    -0.025    -0.282003    -0.225993     0.038311    -0.008585
 3  4     6.224     0.014    -0.732    -0.040    -0.001104    -0.001133     0.002146     0.004701
 3  5     4.988     0.009    -0.732    -0.029    -0.001349    -0.000943     0.002403     0.004230
 3  6     4.988     0.009    -0.732    -0.029    -0.001349    -0.000943     0.002403     0.004230
 3  7     3.752     0.073    -0.732    -0.025    -0.011917    -0.009694    -0.001917     0.004780
 3  8     3.752     0.073    -0.732    -0.025    -0.011917    -0.009694    -0.001917     0.004780
 4  5     3.326     0.041    -0.040    -0.029    -0.005775    -0.006099     0.001143     0.000347
 4  6     3.326     0.041    -0.040    -0.029    -0.005775    -0.006099     0.001143     0.000347
 4  7     4.720     0.003    -0.040    -0.025    -0.000402    -0.000328     0.000325     0.000208
 4  8     4.720     0.003    -0.040    -0.025    -0.000402    -0.000328     0.000325     0.000208
 5  6     3.325     0.040    -0.029    -0.029    -0.005644    -0.006049     0.001173     0.000250
 5  7     4.715     0.004    -0.029    -0.025    -0.000444    -0.000398     0.000285     0.000150
 5  8     5.771     0.011    -0.029    -0.025    -0.001868    -0.000933    -0.024221     0.000122
 7  8     3.330     0.036    -0.025    -0.025    -0.005037    -0.005463     0.001156     0.000180
=====================================================================

 # File: ch3ch2li.wfn
 # Number of Centers:   8
 # Molecule:H (  5)Li(  1)C (  2)
 # Molecular Weight:     36.002499
 # Cartesian coordinates of centers:

        1   C     -1.59773250   -0.35250902    0.00000000
        2   C      1.31425580   -0.27151665    0.00000000
        3   LI     2.99246099    3.11703088    0.00000000
        4   H     -2.37344035   -2.26377603    0.00000000
        5   H     -2.38495925    0.59551327   -1.64839491
        6   H     -2.38495925    0.59551327    1.64839491
        7   H      1.99217949   -1.34557468   -1.63245291
        8   H      1.99217949   -1.34557468    1.63245291

 # Number of Primitives         :  152    reduced to  150
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-----------------------------------------------------------------------------------------------------
 1  2     2.913     1.045     0.183    -0.505    -0.304312    -0.179400     0.004733    -0.031670
 1  3     5.754     0.007     0.183     0.908    -0.000635    -0.000580     0.025802     0.028833
 1  4     2.063     0.960     0.183    -0.099    -0.283034    -0.232736     0.025180    -0.008797
 1  5     2.058     0.967     0.183    -0.107    -0.284267    -0.234855     0.024172    -0.009522
 1  6     2.058     0.967     0.183    -0.107    -0.284267    -0.234855     0.024172    -0.009522
 1  7     4.067     0.055     0.183    -0.136    -0.008256    -0.006784    -0.003521    -0.006105
 1  8     4.067     0.055     0.183    -0.136    -0.008256    -0.006784    -0.003521    -0.006105
 2  3     3.781     0.183    -0.505     0.908    -0.036864    -0.024199    -0.214306    -0.121319
 2  4     4.191     0.062    -0.505    -0.099    -0.007018    -0.007396     0.005948     0.011971
 2  5     4.142     0.051    -0.505    -0.107    -0.007060    -0.006164     0.010172     0.013084
 2  6     4.142     0.051    -0.505    -0.107    -0.007060    -0.006164     0.010172     0.013084
 2  7     2.068     1.041    -0.505    -0.136    -0.292446    -0.251717     0.041142     0.033193
```

```
 2  8     2.068     1.041    -0.505    -0.136    -0.292446    -0.251717     0.041142     0.033193
 3  4     7.599     0.004     0.908    -0.099    -0.000216    -0.000239    -0.009366    -0.011874
 3  5     6.164     0.001     0.908    -0.107    -0.000062    -0.000056    -0.014628    -0.015809
 3  6     6.164     0.001     0.908    -0.107    -0.000062    -0.000056    -0.014628    -0.015809
 3  7     4.856     0.008     0.908    -0.136    -0.000748    -0.000787    -0.020771    -0.025423
 3  8     4.856     0.008     0.908    -0.136    -0.000748    -0.000787    -0.020771    -0.025423
 4  5     3.300     0.049    -0.099    -0.107    -0.007049    -0.007366     0.002480     0.003229
 4  6     3.300     0.049    -0.099    -0.107    -0.007049    -0.007366     0.002480     0.003229
 4  7     4.750     0.005    -0.099    -0.136    -0.000598    -0.000548     0.002334     0.002843
 4  8     4.750     0.005    -0.099    -0.136    -0.000598    -0.000548     0.002334     0.002843
 5  6     3.297     0.050    -0.107    -0.107    -0.007332    -0.007588     0.002662     0.003491
 5  7     4.788     0.004    -0.107    -0.136    -0.000475    -0.000419     0.002475     0.003046
 5  8     5.804     0.014    -0.107    -0.136    -0.001006    -0.001200     0.001604     0.002512
 7  8     3.265     0.058    -0.136    -0.136    -0.008595    -0.008924     0.004006     0.005659
=====================================================================

 # File: ch3cli3.wfn
 # Number of Centers:   8
 # Molecule:H (  3)Li(  3)C (  2)
 # Molecular Weight:     47.868699
 # Cartesian coordinates of centers:

        1   C      0.00000000    0.00000000   -0.06933696
        2   H     -0.94612924    1.63874392   -0.89500377
        3   H     -0.94612924   -1.63874392   -0.89500377
        4   H      1.89225848    0.00000000   -0.89500377
        5   C      0.00000000    0.00000000    2.88507406
        6   LI     1.65594442   -2.86817986    4.47749522
        7   LI     1.65594442    2.86817986    4.47749522
        8   LI    -3.31188883    0.00000000    4.47749522

 # Number of Primitives         :  180    reduced to  178
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.065     0.956     0.192    -0.118    -0.281669    -0.231566     0.022345    -0.010989
 1  3     2.065     0.956     0.192    -0.118    -0.281669    -0.231566     0.022345    -0.010989
 1  4     2.065     0.956     0.192    -0.118    -0.281669    -0.231566     0.022345    -0.010989
 1  5     2.954     1.195     0.192    -2.395    -0.319931    -0.202258    -0.056043    -0.155561
 1  6     5.625     0.010     0.192     0.855    -0.000917    -0.000882     0.025620     0.029165
 1  7     5.625     0.010     0.192     0.855    -0.000917    -0.000882     0.025620     0.029165
 1  8     5.625     0.010     0.192     0.855    -0.000917    -0.000882     0.025620     0.029165
 2  3     3.277     0.050    -0.118    -0.118    -0.007502    -0.007666     0.003207     0.004263
 2  4     3.277     0.050    -0.118    -0.118    -0.007502    -0.007666     0.003207     0.004263
 2  5     4.227     0.085    -0.118    -2.395    -0.009536    -0.010096     0.042112     0.066960
 2  6     7.480     0.004    -0.118     0.855    -0.000244    -0.000294    -0.011064    -0.013509
 2  7     6.095     0.002    -0.118     0.855    -0.000143    -0.000176    -0.022916    -0.016578
 2  8     6.095     0.002    -0.118     0.855    -0.000143    -0.000176    -0.022916    -0.016578
 5  6     3.675     0.285    -2.395     0.855    -0.047205    -0.038725    -0.531571    -0.556979
 5  7     3.675     0.285    -2.395     0.855    -0.047205    -0.038725    -0.531571    -0.556979
 5  8     3.675     0.285    -2.395     0.855    -0.047205    -0.038725    -0.531571    -0.556979
 6  7     5.736     0.006     0.855     0.855    -0.000490    -0.000561     0.130819     0.127370
 6  8     5.736     0.006     0.855     0.855    -0.000490    -0.000561     0.130819     0.127370
=====================================================================

 # File: ch3f.wfn
 # Number of Centers:   5
 # Molecule:H (  3)C (  1)F (  1)
```

```
 # Molecular Weight:     34.033103
 # Cartesian coordinates of centers:

        1   C      0.00000000    0.00000000    0.27870933
        2   H     -0.96705190    1.67498302   -0.37929554
        3   H     -0.96705190   -1.67498302   -0.37929554
        4   H      1.93410380    0.00000000   -0.37929554
        5   F      0.00000000    0.00000000    2.85917729

 # Number of Primitives         :  105    reduced to  103
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.043     0.936     0.760    -0.011    -0.283082    -0.229039     0.044069    -0.004139
 1  3     2.043     0.936     0.760    -0.011    -0.283082    -0.229039     0.044069    -0.004139
 1  4     2.043     0.936     0.760    -0.011    -0.283082    -0.229039     0.044069    -0.004139
 1  5     2.580     0.730     0.760    -0.727    -0.218090    -0.141507    -0.373875    -0.214055
 2  3     3.350     0.037    -0.011    -0.011    -0.004971    -0.005540     0.001291     0.000037
 2  4     3.350     0.037    -0.011    -0.011    -0.004971    -0.005540     0.001291     0.000037
 2  5     3.772     0.073    -0.011    -0.727    -0.011630    -0.009641    -0.004702     0.002142
=====================================================================

 # File: ch3li.wfn
 # Number of Centers:   5
 # Molecule:H (  3)Li(  1)C (  1)
 # Molecular Weight:     21.975700
 # Cartesian coordinates of centers:

        1   C      0.00000004    0.00000000    0.24371023
        2   H     -0.95337330    1.65129099   -0.54750183
        3   H     -0.95337330   -1.65129099   -0.54750183
        4   H      1.90674660    0.00000000   -0.54750183
        5   LI    -0.00000004    0.00000000    3.99879511

 # Number of Primitives         :   95    reduced to   94
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.064     1.063    -0.572    -0.113    -0.294169    -0.257374     0.043115     0.031419
 1  3     2.064     1.063    -0.572    -0.113    -0.294169    -0.257374     0.043115     0.031419
 1  4     2.064     1.063    -0.572    -0.113    -0.294169    -0.257374     0.043115     0.031419
 1  5     3.755     0.180    -0.572     0.912    -0.036446    -0.024019    -0.223892    -0.138988
 2  3     3.303     0.057    -0.113    -0.113    -0.008020    -0.008613     0.002860     0.003890
 2  4     3.303     0.057    -0.113    -0.113    -0.008020    -0.008613     0.002860     0.003890
 2  5     4.930     0.008    -0.113     0.912    -0.000723    -0.000777    -0.015759    -0.020970
=====================================================================

 # File: ch3nh2.wfn
 # Number of Centers:   7
 # Molecule:H (  5)C (  1)N (  1)
 # Molecular Weight:     31.057199
 # Cartesian coordinates of centers:

        1   C     -1.35534554    0.03928302    0.00000000
        2   N      1.38879843    0.13935357    0.00000000
        3   H     -2.13782275   -1.86476141    0.00000000
        4   H     -2.06891962    1.01930849   -1.64906988
        5   H     -2.06891962    1.01930849    1.64906988
        6   H      2.11343367   -0.70006772   -1.52510633
```

```
       7   H      2.11343367   -0.70006772    1.52510633

 # Number of Primitives         :  123    reduced to  121
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.746     0.947     0.600    -1.143    -0.287167    -0.172369    -0.327774    -0.249614
 1  3     2.059     0.943     0.600    -0.076    -0.282056    -0.229083     0.023947    -0.022136
 1  4     2.047     0.942     0.600    -0.041    -0.282249    -0.230008     0.033935    -0.011904
 1  5     2.047     0.942     0.600    -0.041    -0.282249    -0.230008     0.033935    -0.011904
 1  6     3.861     0.020     0.600     0.350    -0.002514    -0.002616     0.077232     0.054387
 1  7     3.861     0.020     0.600     0.350    -0.002514    -0.002616     0.077232     0.054387
 2  3     4.056     0.082    -1.143    -0.076    -0.011032    -0.010113     0.012792     0.021418
 2  4     3.931     0.067    -1.143    -0.041    -0.010573    -0.008461     0.003793     0.011818
 2  5     3.931     0.067    -1.143    -0.041    -0.010573    -0.008461     0.003793     0.011818
 2  6     1.886     0.876    -1.143     0.350    -0.269599    -0.232262    -0.145651    -0.212291
 2  7     1.886     0.876    -1.143     0.350    -0.269599    -0.232262    -0.145651    -0.212291
 3  4     3.323     0.043    -0.076    -0.041    -0.005999    -0.006478     0.001216     0.000929
 3  5     3.323     0.043    -0.076    -0.041    -0.005999    -0.006478     0.001216     0.000929
 3  6     4.664     0.002    -0.076     0.350    -0.000221    -0.000221    -0.004221    -0.005706
 3  7     4.664     0.002    -0.076     0.350    -0.000221    -0.000221    -0.004221    -0.005706
 4  5     3.298     0.041    -0.041    -0.041    -0.005897    -0.006180     0.001168     0.000501
 4  6     4.524     0.002    -0.041     0.350    -0.000232    -0.000218    -0.001716    -0.003146
 4  7     5.525     0.010    -0.041     0.350    -0.000673    -0.000865    -0.008822    -0.002576
 6  7     3.050     0.017     0.350     0.350    -0.002159    -0.002849     0.053873     0.040203
=================================================================

 # File: ch3oh0f.wfn
 # Number of Centers:   6
 # Molecule:H (  4)C (  1)O (  1)
 # Molecular Weight:     32.042000
 # Cartesian coordinates of centers:

       1   C     -1.41084810    0.09216964    0.00000000
       2   H     -2.18058594   -1.79814017    0.00000000
       3   H     -2.09196159    1.07328900   -1.66960964
       4   H     -2.09196159    1.07328900    1.66960964
       5   O      1.22764769   -0.13409352    0.00000000
       6   H      1.69642781   -1.84695015    0.00000000

 # Number of Primitives         :  114    reduced to  112
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.041     0.992     0.181    -0.033    -0.294782    -0.242986     0.032628    -0.002974
 1  3     2.053     0.996     0.181    -0.025    -0.293353    -0.242621     0.033245    -0.002176
 1  4     2.053     0.996     0.181    -0.025    -0.293353    -0.242621     0.033245    -0.002176
 1  5     2.648     0.566     0.181    -0.710    -0.165125    -0.106889    -0.034779    -0.048585
 1  6     3.663     0.014     0.181     0.611    -0.001843    -0.001853     0.057642     0.030261
 2  3     3.323     0.042    -0.033    -0.025    -0.005733    -0.006343     0.001264     0.000248
 2  4     3.323     0.042    -0.033    -0.025    -0.005733    -0.006343     0.001264     0.000248
 2  5     3.793     0.054    -0.033    -0.710    -0.008786    -0.007140     0.002456     0.006262
 2  6     3.877     0.003    -0.033     0.611    -0.000461    -0.000385    -0.002404    -0.005277
 3  4     3.339     0.042    -0.025    -0.025    -0.005684    -0.006314     0.001304     0.000182
 3  5     3.907     0.046    -0.025    -0.710    -0.006850    -0.005896     0.000671     0.004473
 3  6     5.066     0.001    -0.025     0.611    -0.000074    -0.000090     0.000393    -0.002972
 5  6     1.776     0.626    -0.710     0.611    -0.194787    -0.176229    -0.265941    -0.244194
=================================================================
```

```
# File: ch3oh0.wfn
# Number of Centers:   6
# Molecule:H (  4)C (  1)O (  1)
# Molecular Weight:     32.042000
# Cartesian coordinates of centers:

       1   C     -1.41084810    0.09216964    0.00000000
       2   H     -2.18058594   -1.79814017    0.00000000
       3   H     -2.09196159    1.07328900   -1.66960964
       4   H     -2.09196159    1.07328900    1.66960964
       5   O      1.22764769   -0.13409352    0.00000000
       6   H      1.98120951    1.47394308    0.00000000

# Number of Primitives         :  114    reduced to  112
A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
1  2     2.041     0.994     0.182    -0.033    -0.295103    -0.243564     0.032865    -0.002981
1  3     2.053     0.995     0.182    -0.025    -0.293261    -0.242416     0.033170    -0.002215
1  4     2.053     0.995     0.182    -0.025    -0.293261    -0.242416     0.033170    -0.002215
1  5     2.648     0.567     0.182    -0.709    -0.165389    -0.107057    -0.034439    -0.048724
1  6     3.663     0.014     0.182     0.610    -0.001877    -0.001888     0.056506     0.030342
2  3     3.323     0.042    -0.033    -0.025    -0.005745    -0.006366     0.001272     0.000251
2  4     3.323     0.042    -0.033    -0.025    -0.005745    -0.006366     0.001272     0.000251
2  5     3.793     0.050    -0.033    -0.709    -0.007988    -0.006574     0.002264     0.006244
2  6     5.294     0.002    -0.033     0.610    -0.000171    -0.000196    -0.000505    -0.003853
3  4     3.339     0.042    -0.025    -0.025    -0.005680    -0.006309     0.001299     0.000187
3  5     3.907     0.047    -0.025    -0.709    -0.007066    -0.006062     0.000817     0.004530
3  6     4.420     0.001    -0.025     0.610    -0.000107    -0.000109    -0.000274    -0.003449
5  6     1.776     0.627    -0.709     0.610    -0.195100    -0.176671    -0.265851    -0.243593
=================================================================

# File: ch3ohb.wfn
# Number of Centers:   6
# Molecule:H (  4)C (  1)O (  1)
# Molecular Weight:     32.042000
# Cartesian coordinates of centers:

       1   C     -1.39361153    0.07492822    0.00000000
       2   O      1.26157665    0.06733427    0.00000000
       3   H     -2.16889490   -1.82324539    0.00000000
       4   H     -2.07795729    1.05160786   -1.66369082
       5   H     -2.07795729    1.05160786    1.66369082
       6   H      1.89034436   -1.58966197    0.00000000

# Number of Primitives         :  114    reduced to  112
A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
1  2     2.655     0.824     0.747    -1.251    -0.247239    -0.155146    -0.513632    -0.351671
1  3     2.050     0.939     0.747    -0.054    -0.282124    -0.228879     0.029614    -0.019608
1  4     2.047     0.934     0.747    -0.032    -0.281731    -0.228135     0.037337    -0.011619
1  5     2.047     0.934     0.747    -0.032    -0.281731    -0.228135     0.037337    -0.011619
1  6     3.682     0.011     0.747     0.621    -0.001410    -0.001553     0.168471     0.125999
2  3     3.917     0.079    -1.251    -0.054    -0.012015    -0.010058     0.008006     0.017190
2  4     3.859     0.078    -1.251    -0.032    -0.012043    -0.010055     0.000109     0.010323
2  5     3.859     0.078    -1.251    -0.032    -0.012043    -0.010055     0.000109     0.010323
2  6     1.772     0.610    -1.251     0.621    -0.191928    -0.172149    -0.389008    -0.438388
3  4     3.323     0.041    -0.054    -0.032    -0.005649    -0.006097     0.001115     0.000516
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 3  5     3.323     0.041    -0.054    -0.032    -0.005649    -0.006097     0.001115     0.000516
 3  6     4.066     0.003    -0.054     0.621    -0.000402    -0.000385    -0.006119    -0.008227
 4  5     3.327     0.041    -0.032    -0.032    -0.005521    -0.006102     0.001154     0.000305
 4  6     5.049     0.002    -0.032     0.621    -0.000197    -0.000247    -0.000866    -0.003919
=====================================================================

 # File: ch3ohf.wfn
 # Number of Centers:   6
 # Molecule:H (  4)C (  1)O (  1)
 # Molecular Weight:     32.042000
 # Cartesian coordinates of centers:

        1   C     -1.41084810    0.09216964    0.00000000
        2   O      1.22764769   -0.13409352    0.00000000
        3   H     -2.18058594   -1.79814017    0.00000000
        4   H     -2.09196159    1.07328900   -1.66960964
        5   H     -2.09196159    1.07328900    1.66960964
        6   H      1.69642781   -1.84695015    0.00000000

 # Number of Primitives         :  114    reduced to  112
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.648     0.823     0.756    -1.253    -0.247597    -0.155300    -0.522082    -0.357657
 1  3     2.041     0.936     0.756    -0.064    -0.282228    -0.229241     0.026705    -0.023826
 1  4     2.053     0.934     0.756    -0.030    -0.281261    -0.227462     0.037423    -0.011045
 1  5     2.053     0.934     0.756    -0.030    -0.281261    -0.227462     0.037423    -0.011045
 1  6     3.663     0.012     0.756     0.621    -0.001440    -0.001578     0.171053     0.128137
 2  3     3.793     0.086    -1.253    -0.064    -0.013983    -0.011311     0.011173     0.021238
 2  4     3.907     0.076    -1.253    -0.030    -0.011478    -0.009716    -0.000335     0.009612
 2  5     3.907     0.076    -1.253    -0.030    -0.011478    -0.009716    -0.000335     0.009612
 2  6     1.776     0.611    -1.253     0.621    -0.191952    -0.171939    -0.389013    -0.437756
 3  4     3.323     0.041    -0.064    -0.030    -0.005683    -0.006097     0.001076     0.000580
 3  5     3.323     0.041    -0.064    -0.030    -0.005683    -0.006097     0.001076     0.000580
 3  6     3.877     0.004    -0.064     0.621    -0.000501    -0.000459    -0.007825    -0.010294
 4  5     3.339     0.041    -0.030    -0.030    -0.005465    -0.006105     0.001143     0.000269
 4  6     5.066     0.002    -0.030     0.621    -0.000189    -0.000236    -0.000663    -0.003673
=====================================================================

 # File: ch3oh.wfn
 # Number of Centers:   6
 # Molecule:H (  4)C (  1)O (  1)
 # Molecular Weight:     32.042000
 # Cartesian coordinates of centers:

        1   C     -1.41084810    0.09216964    0.00000000
        2   O      1.22764769   -0.13409352    0.00000000
        3   H     -2.18058594   -1.79814017    0.00000000
        4   H     -2.09196159    1.07328900   -1.66960964
        5   H     -2.09196159    1.07328900    1.66960964
        6   H      1.98120951    1.47394308    0.00000000

 # Number of Primitives         :  114    reduced to  112
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.648     0.827     0.751    -1.246    -0.248698    -0.156198    -0.517999    -0.353205
 1  3     2.041     0.932     0.751    -0.015    -0.281538    -0.228272     0.042888    -0.005648
 1  4     2.053     0.935     0.751    -0.052    -0.281447    -0.227783     0.030336    -0.019035
```

```
 1  5     2.053     0.935     0.751    -0.052    -0.281447    -0.227783     0.030336    -0.019035
 1  6     3.663     0.011     0.751     0.614    -0.001408    -0.001560     0.168610     0.125940
 2  3     3.793     0.071    -1.246    -0.015    -0.011845    -0.009360    -0.004841     0.005041
 2  4     3.907     0.082    -1.246    -0.052    -0.012262    -0.010488     0.006820     0.016588
 2  5     3.907     0.082    -1.246    -0.052    -0.012262    -0.010488     0.006820     0.016588
 2  6     1.776     0.618    -1.246     0.614    -0.194022    -0.174089    -0.382829    -0.430832
 3  4     3.323     0.039    -0.015    -0.052    -0.005482    -0.005923     0.001047     0.000240
 3  5     3.323     0.039    -0.015    -0.052    -0.005482    -0.005923     0.001047     0.000240
 3  6     5.294     0.007    -0.015     0.614    -0.000537    -0.000650     0.001291    -0.001781
 4  5     3.339     0.043    -0.052    -0.052    -0.005763    -0.006368     0.001202     0.000811
 4  6     4.420     0.001    -0.052     0.614    -0.000120    -0.000119    -0.004607    -0.007231
=======================================================================

 # File: ch4.wfn
 # Number of Centers:   5
 # Molecule:H (  4)C (  1)
 # Molecular Weight:     16.042600
 # Cartesian coordinates of centers:

        1   C      0.00000000    0.00000000    0.00000000
        2   H      1.18130392   -1.18130392   -1.18130392
        3   H     -1.18130392    1.18130392   -1.18130392
        4   H     -1.18130392   -1.18130392    1.18130392
        5   H      1.18130392    1.18130392    1.18130392

 # Number of Primitives         :   75    reduced to   74
 A  B  distance      delta     QA     QB          Vxc          Vxc(approx)      Vcl          Vcl(approx)
-----------------------------------------------------------------------------------------------------
 1  2     2.046     0.982     0.155    -0.039    -0.287413    -0.240027     0.035040    -0.002937
 1  3     2.046     0.982     0.155    -0.039    -0.287413    -0.240027     0.035040    -0.002937
 1  4     2.046     0.982     0.155    -0.039    -0.287413    -0.240027     0.035040    -0.002937
 1  5     2.046     0.982     0.155    -0.039    -0.287413    -0.240027     0.035040    -0.002937
 2  3     3.341     0.043    -0.039    -0.039    -0.005949    -0.006483     0.001180     0.000449
 2  4     3.341     0.043    -0.039    -0.039    -0.005949    -0.006483     0.001180     0.000449
 2  5     3.341     0.043    -0.039    -0.039    -0.005949    -0.006483     0.001180     0.000449
=======================================================================

 # File: coh2.wfnloc
 # Number of Centers:   4
 # Molecule:H (  2)C (  1)O (  1)
 # Molecular Weight:     30.026200
 # Cartesian coordinates of centers:

        1   C      0.00000000    0.00000000    0.01177397
        2   O      0.00000000    0.00000000   -2.21453747
        3   H      0.00000000    1.75218417    1.10138175
        4   H      0.00000000   -1.75218417    1.10138175

 # Number of Primitives         :  126    reduced to  124
 A  B  distance      delta     QA     QB          Vxc          Vxc(approx)      Vcl          Vcl(approx)
-----------------------------------------------------------------------------------------------------
 1  2     2.226     1.374     1.325    -1.261    -0.405069    -0.308672    -1.128830    -0.750302
 1  3     2.063     0.898     1.325    -0.031    -0.274685    -0.217657     0.039243    -0.020179
 1  4     2.063     0.898     1.325    -0.031    -0.274685    -0.217657     0.039243    -0.020179
 2  3     3.750     0.125    -1.261    -0.031    -0.018430    -0.016667    -0.002658     0.010562
 2  4     3.750     0.125    -1.261    -0.031    -0.018430    -0.016667    -0.002658     0.010562
 3  4     3.504     0.052    -0.031    -0.031    -0.005972    -0.007447     0.000889     0.000282
```

```
======================================================================

 # File: f3.wfn
 # Number of Centers:   3
 # Molecule:F (  3)
 # Molecular Weight:     56.995211
 # Cartesian coordinates of centers:

        1   F      0.00000000    0.00000000    0.00000000
        2   F      0.00000000    0.00000000   -3.13494997
        3   F      0.00000000    0.00000000    3.13494997

 # Number of Primitives         :  108    reduced to  108
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     3.135     0.698     0.156    -0.578    -0.162359    -0.111301    -0.021151    -0.028654
 1  3     3.135     0.698     0.156    -0.578    -0.162359    -0.111301    -0.021151    -0.028654
 2  3     6.270     0.177    -0.578    -0.578    -0.013789    -0.014136     0.044693     0.053216
======================================================================

 # File: h2oh2oh.wfn
 # Number of Centers:   6
 # Molecule:H (  4)O (  2)
 # Molecular Weight:     36.030400
 # Cartesian coordinates of centers:

        1   O     -0.26401035    0.35698104    0.00000000
        2   H      1.52285627    0.28841270    0.00000000
        3   H     -0.71944864    2.07662573    0.00000000
        4   O      5.37764284   -0.02525261    0.00000000
        5   H      6.11688900   -0.77863105   -1.43524223
        6   H      6.11688900   -0.77863105    1.43524223

 # Number of Primitives         :  104    reduced to  104
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     1.788     0.517    -1.292     0.670    -0.166737    -0.144687    -0.434465    -0.483825
 1  3     1.779     0.634    -1.292     0.613    -0.195948    -0.178096    -0.381341    -0.445355
 1  4     5.655     0.047    -1.292    -1.268    -0.006451    -0.004166     0.282845     0.289640
 1  5     6.638     0.001    -1.292     0.638    -0.000040    -0.000042    -0.128290    -0.124193
 1  6     6.638     0.001    -1.292     0.638    -0.000040    -0.000042    -0.128290    -0.124193
 2  3     2.868     0.006     0.670     0.613    -0.000701    -0.000978     0.161281     0.143220
 2  4     3.868     0.045     0.670    -1.268    -0.009660    -0.005852    -0.198989    -0.219558
 2  5     4.930     0.001     0.670     0.638    -0.000065    -0.000065     0.086552     0.086703
 2  6     4.930     0.001     0.670     0.638    -0.000065    -0.000065     0.086552     0.086703
 3  4     6.449     0.001     0.613    -1.268    -0.000069    -0.000064    -0.118775    -0.120571
 3  5     7.546     0.000     0.613     0.638     0.000000    -0.000000     0.054055     0.051868
 3  6     7.546     0.000     0.613     0.638     0.000000    -0.000000     0.054055     0.051868
 4  5     1.782     0.599    -1.268     0.638    -0.186069    -0.168081    -0.398574    -0.454177
 4  6     1.782     0.599    -1.268     0.638    -0.186069    -0.168081    -0.398574    -0.454177
 5  6     2.870     0.006     0.638     0.638    -0.000775    -0.001104     0.160390     0.141892
======================================================================

 # File: h2oh.wfn
 # Number of Centers:   3
 # Molecule:H (  2)O (  1)
 # Molecular Weight:     18.015200
```

```
 # Cartesian coordinates of centers:

        1   O      0.00000000    0.00000000    0.20066456
        2   H     -1.43263141    0.00000000   -0.85622268
        3   H      1.43263141    0.00000000   -0.85622268

 # Number of Primitives         :   52    reduced to   52
 A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     1.780     0.619    -1.247     0.624    -0.191780    -0.173873    -0.379086    -0.436786
 1  3     1.780     0.619    -1.247     0.624    -0.191780    -0.173873    -0.379086    -0.436786
 2  3     2.865     0.007     0.624     0.624    -0.000839    -0.001195     0.154703     0.135736
=======================================================================

 # File: h2onh3h.wfn
 # Number of Centers:   7
 # Molecule:H (  5)N (  1)O (  1)
 # Molecular Weight:     35.045600
 # Cartesian coordinates of centers:

        1   O     -0.23936232   -0.48222801    0.00000000
        2   H      1.37220585   -1.23434468    0.00000000
        3   H      0.00222764    1.29597939    0.00000000
        4   N      0.19150598    5.28111555    0.00000000
        5   H     -1.62714044    5.79702043    0.00000000
        6   H      1.01203941    6.02507488   -1.53102737
        7   H      1.01203941    6.02507488    1.53102737

 # Number of Primitives         :  112    reduced to  112
 A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     1.778     0.640    -1.302     0.608    -0.197764    -0.180038    -0.379004    -0.445385
 1  3     1.795     0.498    -1.302     0.674    -0.160672    -0.138834    -0.444904    -0.488894
 1  4     5.779     0.059    -1.302    -1.093    -0.007886    -0.005105     0.258507     0.246225
 1  5     6.431     0.001    -1.302     0.374    -0.000072    -0.000070    -0.079105    -0.075771
 1  6     6.801     0.001    -1.302     0.370    -0.000076    -0.000077    -0.075530    -0.070841
 1  7     6.801     0.001    -1.302     0.370    -0.000076    -0.000077    -0.075530    -0.070841
 2  3     2.877     0.005     0.608     0.674    -0.000684    -0.000952     0.160589     0.142362
 2  4     6.622     0.001     0.608    -1.093    -0.000091    -0.000083    -0.106178    -0.100341
 2  5     7.644     0.000     0.608     0.374    -0.000001    -0.000001     0.031813     0.029761
 2  6     7.428     0.000     0.608     0.370    -0.000001    -0.000002     0.032008     0.030285
 2  7     7.428     0.000     0.608     0.370    -0.000001    -0.000002     0.032008     0.030285
 3  4     3.990     0.059     0.674    -1.093    -0.012213    -0.007337    -0.185601    -0.184461
 3  5     4.787     0.001     0.674     0.374    -0.000104    -0.000099     0.054087     0.052642
 3  6     5.072     0.001     0.674     0.370    -0.000107    -0.000107     0.050836     0.049123
 3  7     5.072     0.001     0.674     0.370    -0.000107    -0.000107     0.050836     0.049123
 4  5     1.890     0.870    -1.093     0.374    -0.264378    -0.230052    -0.148268    -0.216213
 4  6     1.890     0.873    -1.093     0.370    -0.265496    -0.231090    -0.145855    -0.213871
 4  7     1.890     0.873    -1.093     0.370    -0.265496    -0.231090    -0.145855    -0.213871
 5  6     3.060     0.017     0.374     0.370    -0.002045    -0.002717     0.059037     0.045229
 5  7     3.060     0.017     0.374     0.370    -0.002045    -0.002717     0.059037     0.045229
 6  7     3.062     0.017     0.370     0.370    -0.002069    -0.002748     0.058458     0.044686
=======================================================================

 # File: hffh.wfn
 # Number of Centers:   3
 # Molecule:H (  1)F (  2)
```

```
 # Molecular Weight:     39.004707
 # Cartesian coordinates of centers:

        1   F      0.00000000    0.00000000   -2.12106231
        2   F      0.00000000    0.00000000    2.12106231
        3   H      0.00000000    0.00000000    0.00000000

 # Number of Primitives         :   80    reduced to   80
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     4.242     0.206    -0.896    -0.896    -0.036774    -0.024316     0.189248     0.189055
 1  3     2.121     0.192    -0.896     0.791    -0.060631    -0.045270    -0.314761    -0.333834
=================================================================================

 # File: hfh2oh.wfn
 # Number of Centers:   5
 # Molecule:H (  3)O (  1)F (  1)
 # Molecular Weight:     38.021504
 # Cartesian coordinates of centers:

        1   F     -2.61886659   -0.09028285    0.00000000
        2   H     -0.90087842    0.03519989    0.00000000
        3   O      2.49093370    0.43750362    0.00000000
        4   H      3.35111375    1.03564118   -1.44109655
        5   H      3.35111375    1.03564118    1.44109655

 # Number of Primitives         :   96    reduced to   96
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     1.723     0.315    -0.819     0.799    -0.105016    -0.091326    -0.407492    -0.380200
 1  3     5.137     0.073    -0.819    -1.276    -0.011347    -0.007124     0.210784     0.203542
 1  4     6.244     0.001    -0.819     0.649    -0.000085    -0.000088    -0.093984    -0.085100
 1  5     6.244     0.001    -0.819     0.649    -0.000085    -0.000088    -0.093984    -0.085100
 2  3     3.416     0.052     0.799    -1.276    -0.012445    -0.007624    -0.267606    -0.298722
 2  4     4.600     0.001     0.799     0.649    -0.000087    -0.000090     0.114465     0.112726
 2  5     4.600     0.001     0.799     0.649    -0.000087    -0.000090     0.114465     0.112726
 3  4     1.782     0.584    -1.276     0.649    -0.181974    -0.163878    -0.409839    -0.464616
 3  5     1.782     0.584    -1.276     0.649    -0.181974    -0.163878    -0.409839    -0.464616
 4  5     2.882     0.006     0.649     0.649    -0.000746    -0.001063     0.163985     0.145957
=================================================================================

 # File: hfhfh.wfn
 # Number of Centers:   4
 # Molecule:H (  2)F (  2)
 # Molecular Weight:     40.012607
 # Cartesian coordinates of centers:

        1   F     -2.87070165   -0.24792775    0.00000000
        2   H     -1.17061587   -0.42676452    0.00000000
        3   F      2.43539355    0.08047973    0.00000000
        4   H      3.15941390    1.62616503    0.00000000

 # Number of Primitives         :   88    reduced to   88
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     1.709     0.349    -0.797     0.792    -0.115024    -0.102102    -0.391388    -0.369328
 1  3     5.316     0.045    -0.797    -0.782    -0.006786    -0.004215     0.121150     0.117169
```

```
 1  4     6.315     0.000    -0.797     0.787    -0.000026    -0.000027    -0.108095    -0.099273
 2  3     3.642     0.029     0.792    -0.782    -0.006598    -0.004037    -0.151883    -0.170101
 2  4     4.792     0.000     0.792     0.787    -0.000043    -0.000043     0.130045     0.130085
 3  4     1.707     0.384    -0.782     0.787    -0.122018    -0.112601    -0.380653    -0.360327
=====================================================================

 # File: hfh.wfn
 # Number of Centers:   2
 # Molecule:H (  1)F (  1)
 # Molecular Weight:     20.006304
 # Cartesian coordinates of centers:

        1   F      0.00000000    0.00000000   -0.06851860
        2   H      0.00000000    0.00000000    1.63360515

 # Number of Primitives         :   44    reduced to   44
 A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     1.702     0.407    -0.773     0.773    -0.128957    -0.119683    -0.368620    -0.350898
=====================================================================

 # File: hfn2h.wfn
 # Number of Centers:   4
 # Molecule:H (  1)N (  2)F (  1)
 # Molecular Weight:     48.019703
 # Cartesian coordinates of centers:

        1   F      0.00000000    0.00000000    0.01014936
        2   H      0.00000000    0.00000000    1.71480584
        3   N      0.00000000    0.00000000    6.04879495
        4   N      0.00000000    0.00000000    8.07581824

 # Number of Primitives         :  116    reduced to  116
 A  B  distance      delta    QA    QB          Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------------
 1  2     1.705     0.374    -0.785     0.780    -0.121757    -0.109824    -0.380129    -0.359376
 1  3     6.039     0.027    -0.785    -0.044    -0.003646    -0.002210     0.019260     0.005717
 1  4     8.066     0.001    -0.785     0.049    -0.000105    -0.000090    -0.015196    -0.004759
 2  3     4.334     0.022     0.780    -0.044    -0.004363    -0.002534    -0.026982    -0.007918
 2  4     6.361     0.002     0.780     0.049    -0.000172    -0.000141     0.020013     0.005998
 3  4     2.027     3.036    -0.044     0.049    -0.944578    -0.748963     0.266372    -0.001061
=====================================================================

 # File: hfnh3h.wfn
 # Number of Centers:   6
 # Molecule:H (  4)N (  1)F (  1)
 # Molecular Weight:     37.036703
 # Cartesian coordinates of centers:

        1   F     -0.00000129    0.00000169   -2.57603334
        2   H      0.00000160   -0.00000264   -0.83422756
        3   N      0.00000110    0.00000068    2.58543765
        4   H     -0.88355537    1.53036248    3.25819044
        5   H     -0.88355510   -1.53036263    3.25819044
        6   H      1.76711046    0.00000015    3.25819044

 # Number of Primitives         :  104    reduced to  104
```

A	B	distance	delta	QA	QB	Vxc	Vxc(approx)	Vcl	Vcl(approx)
1	2	1.742	0.297	-0.840	0.795	-0.098936	-0.085128	-0.414732	-0.383425
1	3	5.161	0.104	-0.840	-1.101	-0.015940	-0.010047	0.201762	0.179306
1	4	6.096	0.002	-0.840	0.383	-0.000160	-0.000158	-0.059709	-0.052789
1	5	6.096	0.002	-0.840	0.383	-0.000160	-0.000158	-0.059709	-0.052789
1	6	6.096	0.002	-0.840	0.383	-0.000160	-0.000158	-0.059713	-0.052792
2	3	3.420	0.077	0.795	-1.101	-0.018371	-0.011207	-0.258536	-0.255920
2	4	4.458	0.001	0.795	0.383	-0.000130	-0.000134	0.071958	0.068265
2	5	4.458	0.001	0.795	0.383	-0.000130	-0.000134	0.071958	0.068265
2	6	4.458	0.001	0.795	0.383	-0.000130	-0.000134	0.071963	0.068269
3	4	1.891	0.861	-1.101	0.383	-0.262159	-0.227667	-0.156399	-0.223016
3	5	1.891	0.861	-1.101	0.383	-0.262159	-0.227666	-0.156399	-0.223016
3	6	1.891	0.861	-1.101	0.383	-0.262138	-0.227653	-0.156388	-0.223029
4	5	3.061	0.016	0.383	0.383	-0.001951	-0.002588	0.061699	0.047905
4	6	3.061	0.016	0.383	0.383	-0.001951	-0.002588	0.061703	0.047908
5	6	3.061	0.016	0.383	0.383	-0.001951	-0.002588	0.061703	0.047908

```
# File: li9h9-opt.wfn
# Number of Centers:  18
# Molecule:H (  9)Li(  9)
# Molecular Weight:    71.540100
# Cartesian coordinates of centers:

       1   LI     0.00000000    0.00000000    0.42243226
       2   LI    -3.59973801    0.00000000   -3.66878872
       3   LI     0.00000000   -3.59973801   -3.66878872
       4   LI     3.59973801    0.00000000   -3.66878872
       5   LI     0.00000000    3.59973801   -3.66878872
       6   LI    -3.44529383    3.44529383   -0.18580230
       7   LI    -3.44529383   -3.44529383   -0.18580230
       8   LI     3.44529383   -3.44529383   -0.18580230
       9   LI     3.44529383    3.44529383   -0.18580230
      10   H      0.00000000    0.00000000   -3.51934980
      11   H     -3.76284719    0.00000000    0.32378519
      12   H      0.00000000   -3.76284719    0.32378519
      13   H      3.76284719    0.00000000    0.32378519
      14   H      0.00000000    3.76284719    0.32378519
      15   H     -3.58948687    3.58948687   -3.61113979
      16   H     -3.58948687   -3.58948687   -3.61113979
      17   H      3.58948687   -3.58948687   -3.61113979
      18   H      3.58948687    3.58948687   -3.61113979

# Number of Primitives         :  306    reduced to  306
```

A	B	distance	delta	QA	QB	Vxc	Vxc(approx)	Vcl	Vcl(approx)
1	2	5.449	0.001	0.885	0.889	-0.000118	-0.000092	0.144592	0.144344
1	3	5.449	0.001	0.885	0.889	-0.000118	-0.000092	0.144592	0.144344
1	4	5.449	0.001	0.885	0.889	-0.000118	-0.000092	0.144592	0.144344
1	5	5.449	0.001	0.885	0.889	-0.000118	-0.000092	0.144592	0.144344
1	6	4.910	0.002	0.885	0.891	-0.000275	-0.000215	0.160641	0.160556
1	7	4.910	0.002	0.885	0.891	-0.000275	-0.000215	0.160641	0.160556
1	8	4.910	0.002	0.885	0.891	-0.000275	-0.000215	0.160641	0.160556
1	9	4.910	0.002	0.885	0.891	-0.000275	-0.000215	0.160641	0.160556
1	10	3.942	0.037	0.885	-0.887	-0.006760	-0.004710	-0.198054	-0.199182
1	11	3.764	0.055	0.885	-0.888	-0.009995	-0.007261	-0.204650	-0.208751

```
 1 12     3.764     0.055     0.885    -0.888    -0.009995    -0.007261    -0.204650    -0.208751
 1 13     3.764     0.055     0.885    -0.888    -0.009995    -0.007261    -0.204650    -0.208751
 1 14     3.764     0.055     0.885    -0.888    -0.009995    -0.007261    -0.204650    -0.208751
 1 15     6.484     0.002     0.885    -0.883    -0.000185    -0.000151    -0.120113    -0.120607
 1 16     6.484     0.002     0.885    -0.883    -0.000185    -0.000151    -0.120113    -0.120607
 1 17     6.484     0.002     0.885    -0.883    -0.000185    -0.000151    -0.120113    -0.120607
 1 18     6.484     0.002     0.885    -0.883    -0.000185    -0.000151    -0.120113    -0.120607
 2  3     5.091     0.002     0.889     0.889    -0.000271    -0.000218     0.155548     0.155138
 2  4     7.199     0.001     0.889     0.889    -0.000052    -0.000043     0.109959     0.109699
 2  5     5.091     0.002     0.889     0.889    -0.000271    -0.000218     0.155548     0.155138
 2  6     4.902     0.003     0.889     0.891    -0.000323    -0.000262     0.161617     0.161490
 2  7     4.902     0.003     0.889     0.891    -0.000323    -0.000262     0.161617     0.161490
 2  8     8.581     0.000     0.889     0.891    -0.000004    -0.000004     0.092336     0.092244
 2  9     8.581     0.000     0.889     0.891    -0.000004    -0.000004     0.092336     0.092244
 2 10     3.603     0.054     0.889    -0.887    -0.010328    -0.007491    -0.212895    -0.218801
 2 11     3.996     0.041     0.889    -0.888    -0.007136    -0.005158    -0.194902    -0.197439
 2 12     6.562     0.002     0.889    -0.888    -0.000186    -0.000156    -0.119064    -0.120232
 2 13     8.375     0.001     0.889    -0.888    -0.000036    -0.000033    -0.093534    -0.094197
 2 14     6.562     0.002     0.889    -0.888    -0.000186    -0.000156    -0.119064    -0.120232
 2 15     3.590     0.077     0.889    -0.883    -0.013816    -0.010660    -0.211535    -0.218705
 2 16     3.590     0.077     0.889    -0.883    -0.013816    -0.010660    -0.211535    -0.218705
 2 17     8.036     0.001     0.889    -0.883    -0.000066    -0.000059    -0.097184    -0.097707
 2 18     8.036     0.001     0.889    -0.883    -0.000066    -0.000059    -0.097184    -0.097707
 6  7     6.891     0.001     0.891     0.891    -0.000118    -0.000098     0.115202     0.115132
 6  8     9.745     0.000     0.891     0.891    -0.000002    -0.000002     0.081421     0.081411
 6  9     6.891     0.001     0.891     0.891    -0.000118    -0.000098     0.115202     0.115132
 6 10     5.904     0.003     0.891    -0.887    -0.000334    -0.000263    -0.132946    -0.133830
 6 11     3.497     0.076     0.891    -0.888    -0.013968    -0.010806    -0.214434    -0.226099
 6 12     8.005     0.001     0.891    -0.888    -0.000071    -0.000062    -0.098056    -0.098773
 6 13     8.005     0.001     0.891    -0.888    -0.000071    -0.000062    -0.098056    -0.098773
 6 14     3.497     0.076     0.891    -0.888    -0.013968    -0.010806    -0.214434    -0.226099
 6 15     3.431     0.092     0.891    -0.883    -0.016966    -0.013346    -0.220673    -0.229325
 6 16     7.826     0.001     0.891    -0.883    -0.000080    -0.000068    -0.100130    -0.100554
 6 17    10.522     0.000     0.891    -0.883    -0.000006    -0.000006    -0.074464    -0.074788
 6 18     7.826     0.001     0.891    -0.883    -0.000080    -0.000068    -0.100130    -0.100554
10 11     5.379     0.052    -0.887    -0.888    -0.007562    -0.004796     0.144372     0.146411
10 12     5.379     0.052    -0.887    -0.888    -0.007562    -0.004796     0.144372     0.146411
10 13     5.379     0.052    -0.887    -0.888    -0.007562    -0.004796     0.144372     0.146411
10 14     5.379     0.052    -0.887    -0.888    -0.007562    -0.004796     0.144372     0.146411
10 15     5.077     0.080    -0.887    -0.883    -0.011776    -0.007843     0.151464     0.154355
10 16     5.077     0.080    -0.887    -0.883    -0.011776    -0.007843     0.151464     0.154355
10 17     5.077     0.080    -0.887    -0.883    -0.011776    -0.007843     0.151464     0.154355
10 18     5.077     0.080    -0.887    -0.883    -0.011776    -0.007843     0.151464     0.154355
11 12     5.321     0.067    -0.888    -0.888    -0.009431    -0.006332     0.144389     0.148102
11 13     7.526     0.004    -0.888    -0.888    -0.000266    -0.000238     0.103315     0.104724
11 14     5.321     0.067    -0.888    -0.888    -0.009431    -0.006332     0.144389     0.148102
11 15     5.329     0.073    -0.888    -0.883    -0.010117    -0.006850     0.144562     0.147180
11 16     5.329     0.073    -0.888    -0.883    -0.010117    -0.006850     0.144562     0.147180
11 17     9.079     0.002    -0.888    -0.883    -0.000107    -0.000103     0.085308     0.086390
11 18     9.079     0.002    -0.888    -0.883    -0.000107    -0.000103     0.085308     0.086390
15 16     7.179     0.007    -0.883    -0.883    -0.000548    -0.000455     0.107463     0.108725
15 17    10.153     0.001    -0.883    -0.883    -0.000074    -0.000069     0.076143     0.076880
15 18     7.179     0.007    -0.883    -0.883    -0.000548    -0.000455     0.107463     0.108725
=====================================================================


 # File: lih.wfn
 # Number of Centers:   3
```

```
 # Molecule:H (  1)Li(  1)
 # Molecular Weight:      7.948900
 # Cartesian coordinates of centers:

        1   LI     0.00000000    0.00000000   -0.10306550
        2   H      0.00000000    0.00000000    2.93765448
        3   X      0.00000000    0.00000000   -6.28200654

 # Number of Primitives         :   38    reduced to   38
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     3.041     0.198     0.911    -0.911    -0.035736    -0.032545    -0.253752    -0.273037
 1  3     6.179     0.000     0.911     0.000     0.000000    -0.000000     0.000000     0.000000
 2  3     9.220     0.000    -0.911     0.000     0.000000    -0.000000     0.000000    -0.000000
=================================================================

 # File: n5+.wfn
 # Number of Centers:   5
 # Molecule:N (  5)
 # Molecular Weight:     70.033498
 # Cartesian coordinates of centers:

        1   N      0.00000000    0.00000000   -0.65253239
        2   N      2.02260219    0.00000000   -2.12412132
        3   N     -2.02260219    0.00000000   -2.12412132
        4   N      3.86962309    0.00000000   -2.95948317
        5   N     -3.86962309    0.00000000   -2.95948317

 # Number of Primitives         :  180    reduced to  180
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.501     1.234     0.160    -0.313    -0.402379    -0.246705     0.038281    -0.020046
 1  3     2.501     1.234     0.160    -0.313    -0.402379    -0.246705     0.038281    -0.020046
 1  4     4.505     0.183     0.160     0.737    -0.018360    -0.020277     0.080795     0.026196
 1  5     4.505     0.183     0.160     0.737    -0.018360    -0.020277     0.080795     0.026196
 2  3     4.045     0.110    -0.313    -0.313    -0.021175    -0.013551     0.018677     0.024204
 2  4     2.027     2.602    -0.313     0.737    -0.839996    -0.641738    -0.119643    -0.113686
 2  5     5.951     0.034    -0.313     0.737    -0.002958    -0.002851    -0.038400    -0.038725
 4  5     7.739     0.020     0.737     0.737    -0.001246    -0.001319     0.101625     0.070090
=================================================================

 # File: nh3h2oh.wfn
 # Number of Centers:   7
 # Molecule:H (  5)N (  1)O (  1)
 # Molecular Weight:     35.045600
 # Cartesian coordinates of centers:

        1   N      0.19156807    0.21948033    0.00000000
        2   H      0.37779602    2.10075140    0.00000000
        3   H      1.04994146   -0.47758751   -1.53044986
        4   H      1.04994146   -0.47758751    1.53044986
        5   O     -0.23838134    6.51351009    0.00000000
        6   H     -1.21543284    6.92664103   -1.43089124
        7   H     -1.21543284    6.92664103    1.43089124

 # Number of Primitives         :  112    reduced to  112
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
```

```
-------------------------------------------------------------------------------------------------
 1  2     1.890     0.821    -1.105     0.404    -0.254590    -0.217048    -0.164893    -0.235876
 1  3     1.888     0.893    -1.105     0.349    -0.270522    -0.236512    -0.133076    -0.204293
 1  4     1.888     0.893    -1.105     0.349    -0.270522    -0.236512    -0.133076    -0.204293
 1  5     6.309     0.027    -1.105    -1.257    -0.003276    -0.002115     0.212431     0.220090
 1  6     7.001     0.000    -1.105     0.630    -0.000013    -0.000013    -0.099623    -0.099377
 1  7     7.001     0.000    -1.105     0.630    -0.000013    -0.000013    -0.099623    -0.099377
 2  3     3.073     0.016     0.404     0.349    -0.001955    -0.002566     0.059435     0.045876
 2  4     3.073     0.016     0.404     0.349    -0.001955    -0.002566     0.059435     0.045876
 2  5     4.456     0.035     0.404    -1.257    -0.006617    -0.003959    -0.103928    -0.113886
 2  6     5.280     0.000     0.404     0.630    -0.000039    -0.000038     0.046746     0.048158
 2  7     5.280     0.000     0.404     0.630    -0.000039    -0.000038     0.046746     0.048158
 3  4     3.061     0.018     0.349     0.349    -0.002227    -0.002960     0.053532     0.039838
 3  5     7.272     0.001     0.349    -1.257    -0.000076    -0.000067    -0.062032    -0.060363
 3  6     7.744     0.000     0.349     0.630     0.000000    -0.000000     0.029778     0.028403
 3  7     8.290     0.000     0.349     0.630     0.000000    -0.000000     0.026935     0.026531
 5  6     1.781     0.611    -1.257     0.630    -0.189284    -0.171427    -0.388620    -0.444473
 5  7     1.781     0.611    -1.257     0.630    -0.189284    -0.171427    -0.388620    -0.444473
 6  7     2.862     0.007     0.630     0.630    -0.000803    -0.001144     0.157450     0.138621
=================================================================================

 # File: nh3h.wfn
 # Number of Centers:   4
 # Molecule:H (  3)N (  1)
 # Molecular Weight:     17.030400
 # Cartesian coordinates of centers:

        1   N      0.00000000    0.00000000    2.63044045
        2   H     -0.88607879    1.53473349    3.28066993
        3   H     -0.88607879   -1.53473349    3.28066993
        4   H      1.77215759    0.00000000    3.28066993

 # Number of Primitives         :   60    reduced to   60
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     1.888     0.884    -1.077     0.359    -0.268208    -0.234028    -0.134984    -0.204917
 1  3     1.888     0.884    -1.077     0.359    -0.268208    -0.234028    -0.134984    -0.204917
 1  4     1.888     0.883    -1.077     0.359    -0.268175    -0.234009    -0.134952    -0.204921
 2  3     3.069     0.018     0.359     0.359    -0.002149    -0.002866     0.055717     0.042007
 2  4     3.069     0.018     0.359     0.359    -0.002150    -0.002866     0.055718     0.042008
 3  4     3.069     0.018     0.359     0.359    -0.002150    -0.002866     0.055718     0.042008
=================================================================================

 # File: nh3nh3h.wfn
 # Number of Centers:   8
 # Molecule:H (  6)N (  2)
 # Molecular Weight:     34.060799
 # Cartesian coordinates of centers:

        1   N     -0.65108508   -0.81393859    0.00000000
        2   H      0.12083161   -1.60456354   -1.53114564
        3   H      0.12083161   -1.60456354    1.53114564
        4   H     -0.25136017    1.03590827    0.00000000
        5   N      0.07490087    5.62374987    0.00000000
        6   H      1.72329675    6.54584969    0.00000000
        7   H     -0.90087921    6.14917377   -1.53003489
        8   H     -0.90087921    6.14917377    1.53003489
```

```
 # Number of Primitives         :  120    reduced to  120
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     1.888     0.897    -1.112     0.345    -0.271455    -0.237502    -0.131737    -0.203277
 1  3     1.888     0.897    -1.112     0.345    -0.271455    -0.237502    -0.131737    -0.203277
 1  4     1.893     0.805    -1.112     0.413    -0.250382    -0.212562    -0.173275    -0.242439
 1  5     6.478     0.030    -1.112    -1.083    -0.003527    -0.002300     0.188580     0.185875
 1  6     7.733     0.001    -1.112     0.362    -0.000032    -0.000033    -0.053916    -0.052088
 1  7     7.134     0.000    -1.112     0.365    -0.000028    -0.000027    -0.058028    -0.056852
 1  8     7.134     0.000    -1.112     0.365    -0.000028    -0.000027    -0.058028    -0.056852
 2  3     3.062     0.018     0.345     0.345    -0.002259    -0.003000     0.052599     0.038920
 2  4     3.075     0.015     0.345     0.413    -0.001919    -0.002520     0.060060     0.046334
 2  5     7.389     0.001     0.345    -1.083    -0.000084    -0.000073    -0.054579    -0.050606
 2  6     8.446     0.000     0.345     0.362    -0.000001    -0.000001     0.015922     0.014809
 2  7     7.821     0.000     0.345     0.365    -0.000001    -0.000001     0.017098     0.016102
 2  8     8.399     0.000     0.345     0.365    -0.000001    -0.000001     0.011442     0.014995
 4  5     4.599     0.044     0.413    -1.083    -0.008107    -0.004815    -0.095631    -0.097182
 4  6     5.853     0.001     0.413     0.362    -0.000090    -0.000088     0.025715     0.025545
 4  7     5.377     0.001     0.413     0.365    -0.000077    -0.000071     0.027886     0.027998
 4  8     5.377     0.001     0.413     0.365    -0.000077    -0.000071     0.027886     0.027998
 5  6     1.889     0.880    -1.083     0.362    -0.267398    -0.232986    -0.138990    -0.207760
 5  7     1.889     0.878    -1.083     0.365    -0.266784    -0.232484    -0.140422    -0.209125
 5  8     1.889     0.878    -1.083     0.365    -0.266784    -0.232484    -0.140422    -0.209125
 6  7     3.063     0.017     0.362     0.365    -0.002121    -0.002821     0.056911     0.043141
 6  8     3.063     0.017     0.362     0.365    -0.002121    -0.002821     0.056911     0.043141
 7  8     3.060     0.017     0.365     0.365    -0.002103    -0.002797     0.057297     0.043483
=================================================================================

 # File: pentane.wfn
 # Number of Centers:  17
 # Molecule:H ( 12)C (  5)
 # Molecular Weight:     72.149798
 # Cartesian coordinates of centers:

       1   C      0.00000000    0.00000000    0.06334947
       2   C     -2.41414962    0.00000000   -1.52056579
       3   C      2.41414962    0.00000000   -1.52056579
       4   C     -4.81771425    0.00000000    0.07657448
       5   C      4.81771425    0.00000000    0.07657448
       6   H      0.00000000   -1.64546078    1.29676852
       7   H      0.00000000    1.64546078    1.29676852
       8   H     -2.41683372   -1.64423797   -2.75237434
       9   H      2.41683372   -1.64423797   -2.75237434
      10   H     -2.41683372    1.64423797   -2.75237434
      11   H      2.41683372    1.64423797   -2.75237434
      12   H     -4.90312174   -1.65663532    1.28367381
      13   H      4.90312174   -1.65663532    1.28367381
      14   H     -4.90312174    1.65663532    1.28367381
      15   H      4.90312174    1.65663532    1.28367381
      16   H     -6.49306837    0.00000000   -1.10444806
      17   H      6.49306837    0.00000000   -1.10444806

 # Number of Primitives         :  303    reduced to  298
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.887     0.969     0.148     0.163    -0.299051    -0.167849     0.026058     0.008353
```

1	3	2.887	0.969	0.148	0.163	-0.299051	-0.167849	0.026058	0.008353
1	4	4.818	0.045	0.148	0.161	-0.006965	-0.004619	0.005657	0.004931
1	5	4.818	0.045	0.148	0.161	-0.006965	-0.004619	0.005657	0.004931
1	6	2.056	0.944	0.148	-0.076	-0.282400	-0.229563	0.027366	-0.005437
1	7	2.056	0.944	0.148	-0.076	-0.282400	-0.229563	0.027366	-0.005437
1	8	4.059	0.042	0.148	-0.073	-0.006400	-0.005230	-0.000817	-0.002658
1	9	4.059	0.042	0.148	-0.073	-0.006400	-0.005230	-0.000817	-0.002658
1	10	4.059	0.042	0.148	-0.073	-0.006400	-0.005230	-0.000817	-0.002658
1	11	4.059	0.042	0.148	-0.073	-0.006400	-0.005230	-0.000817	-0.002658
1	12	5.317	0.007	0.148	-0.060	-0.000894	-0.000633	-0.001344	-0.001676
1	13	5.317	0.007	0.148	-0.060	-0.000894	-0.000633	-0.001344	-0.001676
1	14	5.317	0.007	0.148	-0.060	-0.000894	-0.000633	-0.001344	-0.001676
1	15	5.317	0.007	0.148	-0.060	-0.000894	-0.000633	-0.001344	-0.001676
1	16	6.597	0.010	0.148	-0.057	-0.000788	-0.000787	-0.000775	-0.001280
1	17	6.597	0.010	0.148	-0.057	-0.000788	-0.000787	-0.000775	-0.001280
2	3	4.828	0.042	0.163	0.163	-0.006616	-0.004352	0.006234	0.005503
2	4	2.886	0.980	0.163	0.161	-0.299828	-0.169811	0.028156	0.009069
2	5	7.406	0.009	0.163	0.161	-0.000721	-0.000621	0.003515	0.003534
2	6	4.059	0.041	0.163	-0.076	-0.006230	-0.005085	-0.001154	-0.003035
2	7	4.059	0.041	0.163	-0.076	-0.006230	-0.005085	-0.001154	-0.003035
2	8	2.054	0.948	0.163	-0.073	-0.283426	-0.230778	0.027720	-0.005785
2	9	5.250	0.007	0.163	-0.073	-0.001000	-0.000681	-0.001900	-0.002264
2	10	2.054	0.948	0.163	-0.073	-0.283426	-0.230778	0.027720	-0.005785
2	11	5.250	0.007	0.163	-0.073	-0.001000	-0.000681	-0.001900	-0.002264
2	12	4.099	0.041	0.163	-0.060	-0.005881	-0.005014	-0.000451	-0.002395
2	13	8.009	0.001	0.163	-0.060	-0.000051	-0.000046	-0.001065	-0.001226
2	14	4.099	0.041	0.163	-0.060	-0.005881	-0.005014	-0.000451	-0.002395
2	15	8.009	0.001	0.163	-0.060	-0.000051	-0.000046	-0.001065	-0.001226
2	16	4.100	0.042	0.163	-0.057	-0.006030	-0.005063	-0.000441	-0.002269
2	17	8.917	0.002	0.163	-0.057	-0.000101	-0.000106	-0.000793	-0.001043
4	5	9.635	0.002	0.161	0.161	-0.000087	-0.000083	0.002602	0.002675
4	6	5.235	0.008	0.161	-0.076	-0.001066	-0.000718	-0.001887	-0.002318
4	7	5.235	0.008	0.161	-0.076	-0.001066	-0.000718	-0.001887	-0.002318
4	8	4.058	0.043	0.161	-0.073	-0.006588	-0.005357	-0.001031	-0.002884
4	9	7.940	0.001	0.161	-0.073	-0.000056	-0.000050	-0.001326	-0.001474
4	10	4.058	0.043	0.161	-0.073	-0.006588	-0.005357	-0.001031	-0.002884
4	11	7.940	0.001	0.161	-0.073	-0.000056	-0.000050	-0.001326	-0.001474
4	12	2.052	0.964	0.161	-0.060	-0.285153	-0.234826	0.030729	-0.004713
4	13	9.935	0.000	0.161	-0.060	-0.000003	-0.000003	-0.000907	-0.000973
4	14	2.052	0.964	0.161	-0.060	-0.285153	-0.234826	0.030729	-0.004713
4	15	9.935	0.000	0.161	-0.060	-0.000003	-0.000003	-0.000907	-0.000973
4	16	2.050	0.967	0.161	-0.057	-0.285993	-0.235890	0.031264	-0.004470
4	17	11.372	0.000	0.161	-0.057	-0.000017	-0.000017	-0.000638	-0.000806
6	7	3.291	0.044	-0.076	-0.076	-0.006492	-0.006617	0.001661	0.001735
6	8	4.716	0.004	-0.076	-0.073	-0.000435	-0.000375	0.000991	0.001168
6	9	4.716	0.004	-0.076	-0.073	-0.000435	-0.000375	0.000991	0.001168
6	10	5.750	0.011	-0.076	-0.073	-0.000829	-0.000991	0.000527	0.000958
6	11	5.750	0.011	-0.076	-0.073	-0.000829	-0.000991	0.000527	0.000958
6	12	4.903	0.006	-0.076	-0.060	-0.001039	-0.000656	0.001114	0.000928
6	13	4.903	0.006	-0.076	-0.060	-0.001039	-0.000656	0.001114	0.000928
6	14	5.911	0.001	-0.076	-0.060	-0.000049	-0.000043	0.000584	0.000770
6	15	5.911	0.001	-0.076	-0.060	-0.000049	-0.000043	0.000584	0.000770
6	16	7.116	0.001	-0.076	-0.057	-0.000060	-0.000057	0.000374	0.000606
6	17	7.116	0.001	-0.076	-0.057	-0.000060	-0.000057	0.000374	0.000606
8	9	4.834	0.007	-0.073	-0.073	-0.001171	-0.000737	0.001302	0.001100
8	10	3.288	0.043	-0.073	-0.073	-0.006450	-0.006595	0.001592	0.001616
8	11	5.846	0.001	-0.073	-0.073	-0.000054	-0.000047	0.000719	0.000909

```
 8 12     4.740     0.004    -0.073    -0.060    -0.000430    -0.000373     0.000804     0.000926
 8 13     8.359     0.000    -0.073    -0.060    -0.000003    -0.000003     0.000466     0.000525
 8 14     5.776     0.012    -0.073    -0.060    -0.000853    -0.001011     0.000393     0.000760
 8 15     8.987     0.000    -0.073    -0.060    -0.000021    -0.000021     0.000345     0.000489
 8 16     4.694     0.004    -0.073    -0.057    -0.000474    -0.000393     0.000818     0.000886
 8 17     9.209     0.000    -0.073    -0.057    -0.000003    -0.000003     0.000370     0.000452
12 13     9.806     0.000    -0.060    -0.060    -0.000001    -0.000001     0.000369     0.000370
12 14     3.313     0.044    -0.060    -0.060    -0.006279    -0.006622     0.001348     0.001095
12 15    10.351     0.000    -0.060    -0.060     0.000000    -0.000000     0.000307     0.000350
12 16     3.313     0.043    -0.060    -0.057    -0.006237    -0.006559     0.001315     0.001037
12 17    11.761     0.000    -0.060    -0.057    -0.000001    -0.000001     0.000222     0.000292
16 17    12.986     0.000    -0.057    -0.057    -0.000005    -0.000006     0.000189     0.000251
=====================================================================


 # File: propane.wfn
 # Number of Centers:  11
 # Molecule:H (  8)C (  3)
 # Molecular Weight:     44.096199
 # Cartesian coordinates of centers:

        1   C     -2.64888283   -0.91361062    0.00000000
        2   C      0.23550922   -0.82843725    0.00000000
        3   C      1.27864280    1.86208166    0.00000000
        4   H     -3.33603742   -2.84494956    0.00000000
        5   H     -3.41391895    0.02428240   -1.65662414
        6   H     -3.41391895    0.02428240    1.65662414
        7   H      0.94553332   -1.83309250   -1.64350954
        8   H      0.94553332   -1.83309250    1.64350954
        9   H      3.32856252    1.86512852    0.00000000
       10   H      0.64990823    2.89631326   -1.65662580
       11   H      0.64990823    2.89631326    1.65662580

 # Number of Primitives         :  189    reduced to  186
 A  B  distance      delta    QA    QB         Vxc         Vxc(approx)      Vcl         Vcl(approx)
-------------------------------------------------------------------------------------------------
 1  2     2.886     0.980     0.160     0.174    -0.299878    -0.169863     0.028625     0.009652
 1  3     4.809     0.046     0.160     0.160    -0.007229    -0.004811     0.005847     0.005341
 1  4     2.050     0.967     0.160    -0.057    -0.285948    -0.235856     0.031263    -0.004453
 1  5     2.052     0.964     0.160    -0.060    -0.285120    -0.234824     0.030728    -0.004696
 1  6     2.052     0.964     0.160    -0.060    -0.285120    -0.234824     0.030728    -0.004696
 1  7     4.058     0.044     0.160    -0.070    -0.006601    -0.005402    -0.000921    -0.002771
 1  8     4.058     0.044     0.160    -0.070    -0.006601    -0.005402    -0.000921    -0.002771
 1  9     6.592     0.011     0.160    -0.057    -0.000810    -0.000813    -0.000844    -0.001386
 1 10     5.305     0.007     0.160    -0.060    -0.000943    -0.000658    -0.001376    -0.001814
 1 11     5.305     0.007     0.160    -0.060    -0.000943    -0.000658    -0.001376    -0.001814
 2  3     2.886     0.980     0.174     0.160    -0.299835    -0.169845     0.028640     0.009654
 2  4     4.101     0.041     0.174    -0.057    -0.006013    -0.005051    -0.000494    -0.002414
 2  5     4.098     0.041     0.174    -0.060    -0.005906    -0.005035    -0.000550    -0.002550
 2  6     4.098     0.041     0.174    -0.060    -0.005906    -0.005035    -0.000550    -0.002550
 2  7     2.053     0.953     0.174    -0.070    -0.284421    -0.232006     0.028111    -0.005940
 2  8     2.053     0.953     0.174    -0.070    -0.284421    -0.232006     0.028111    -0.005940
 2  9     4.101     0.041     0.174    -0.057    -0.006009    -0.005048    -0.000501    -0.002416
 2 10     4.098     0.041     0.174    -0.060    -0.005902    -0.005032    -0.000548    -0.002547
 2 11     4.098     0.041     0.174    -0.060    -0.005902    -0.005032    -0.000548    -0.002547
 3  4     6.592     0.011     0.160    -0.057    -0.000808    -0.000812    -0.000841    -0.001385
 3  5     5.305     0.007     0.160    -0.060    -0.000936    -0.000654    -0.001381    -0.001816
 3  6     5.305     0.007     0.160    -0.060    -0.000936    -0.000654    -0.001381    -0.001816
```

3	7	4.058	0.044	0.160	-0.070	-0.006606	-0.005405	-0.000917	-0.002771
3	8	4.058	0.044	0.160	-0.070	-0.006606	-0.005405	-0.000917	-0.002771
3	9	2.050	0.967	0.160	-0.057	-0.286015	-0.235898	0.031250	-0.004459
3	10	2.052	0.963	0.160	-0.060	-0.285072	-0.234792	0.030738	-0.004692
3	11	2.052	0.963	0.160	-0.060	-0.285072	-0.234792	0.030738	-0.004692
4	5	3.314	0.043	-0.057	-0.060	-0.006219	-0.006542	0.001311	0.001033
4	6	3.314	0.043	-0.057	-0.060	-0.006219	-0.006542	0.001311	0.001033
4	7	4.696	0.004	-0.057	-0.070	-0.000471	-0.000391	0.000787	0.000851
4	8	4.696	0.004	-0.057	-0.070	-0.000471	-0.000391	0.000787	0.000851
4	9	8.161	0.002	-0.057	-0.057	-0.000123	-0.000143	0.000269	0.000398
4	10	7.183	0.001	-0.057	-0.060	-0.000054	-0.000053	0.000292	0.000476
4	11	7.183	0.001	-0.057	-0.060	-0.000054	-0.000053	0.000292	0.000476
5	6	3.313	0.044	-0.060	-0.060	-0.006288	-0.006631	0.001346	0.001091
5	7	4.739	0.004	-0.060	-0.070	-0.000432	-0.000375	0.000777	0.000890
5	8	5.775	0.012	-0.060	-0.070	-0.000865	-0.001028	0.000375	0.000730
5	9	7.183	0.001	-0.060	-0.057	-0.000054	-0.000053	0.000293	0.000477
5	10	4.976	0.006	-0.060	-0.060	-0.000912	-0.000580	0.000898	0.000725
5	11	5.978	0.000	-0.060	-0.060	-0.000044	-0.000039	0.000438	0.000604
7	8	3.287	0.043	-0.070	-0.070	-0.006410	-0.006578	0.001523	0.001498
7	9	4.696	0.004	-0.070	-0.057	-0.000471	-0.000391	0.000788	0.000852
7	10	4.739	0.004	-0.070	-0.060	-0.000432	-0.000375	0.000777	0.000889
7	11	5.775	0.012	-0.070	-0.060	-0.000865	-0.001028	0.000374	0.000730
9	10	3.314	0.043	-0.057	-0.060	-0.006219	-0.006542	0.001311	0.001033
9	11	3.314	0.043	-0.057	-0.060	-0.006219	-0.006542	0.001311	0.001033
10	11	3.313	0.044	-0.060	-0.060	-0.006285	-0.006629	0.001345	0.001088

CORRELATED DATA:

MOLECULE & CALCULATION = HNC CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	0.00000000	0.00000000	2.68019856
2	N	0.00000000	0.00000000	0.81655066
3	C	0.00000000	0.00000000	-1.39934220

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.559161	-1.565742	1.863648	0.599685	0.875502	1.175344
1	3	0.559161	1.006306	4.079541	0.039679	-0.562687	-0.542848
2	3	-1.565742	1.006306	2.215893	1.400243	1.575616	2.275737

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-124.39	-100.96	-203.45	-294.79	-327.84	-395.75
1	3	-2.16	-3.05	133.19	86.55	131.03	83.50
2	3	-276.45	-198.26	-825.59	-446.19	-1102.04	-644.46

MOLECULE & CALCULATION = FCN CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	0.27873460
2	F	0.00000000	0.00000000	-2.10609977
3	N	0.00000000	0.00000000	2.46892718

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	1.740847	-0.601388	2.384834	0.792706	1.046924	1.443277
1	3	1.740847	-1.139190	2.190193	1.601654	1.983155	2.783982
2	3	-0.601388	-1.139190	4.575027	0.177346	-0.685095	-0.596422

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-175.11	-104.29	-364.80	-275.47	-539.91	-379.76
1	3	-342.87	-229.44	-666.57	-568.19	-1009.45	-797.64
2	3	-12.42	-12.16	113.75	93.97	101.33	81.81

MOLECULE & CALCULATION = HF_CO CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	0.00000000	0.00000000	-2.19392338
2	F	0.00000000	0.00000000	-3.89925263
3	O	0.00000000	0.00000000	1.82222569
4	C	0.00000000	0.00000000	3.92433676

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.730387	-0.736783	1.705329	0.417175	0.538137	0.746724
1	3	0.730387	-1.232320	4.016149	0.033328	0.900071	0.916735
1	4	0.730387	1.238148	6.118260	-0.004740	-0.904327	-0.906697
2	3	-0.736783	-1.232320	5.721478	0.016093	-0.907952	-0.899906
2	4	-0.736783	1.238148	7.823589	0.010623	0.912246	0.917558
3	4	-1.232320	1.238148	2.102111	1.320936	1.525795	2.186263

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-90.26	-76.75	-203.20	-198.02	-293.46	-274.77
1	3	-4.72	-2.60	-112.50	-140.63	-117.22	-143.24
1	4	0.22	0.24	109.72	92.75	109.94	92.99
2	3	-1.96	-0.88	94.14	99.58	92.18	98.70
2	4	-0.33	-0.43	-92.64	-73.17	-92.97	-73.59
3	4	-267.12	-197.16	-866.94	-455.47	-1134.06	-652.63

MOLECULE & CALCULATION = HCN_HF CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	-3.60567618
2	H	0.00000000	0.00000000	-5.61823451
3	N	0.00000000	0.00000000	-1.42757785
4	H	0.00000000	0.00000000	2.16290178
5	F	0.00000000	0.00000000	3.89804831

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	1.056213	0.215614	2.012558	0.788209	-0.227734	0.166370
1	3	1.056213	-1.239831	2.178098	1.614693	1.309526	2.116872
1	4	1.056213	0.735881	5.768578	-0.002607	-0.777247	-0.778551
1	5	1.056213	-0.767014	7.503724	0.014717	0.810130	0.817489
2	3	0.215614	-1.239831	4.190657	0.084629	0.267325	0.309639

2	4	0.215614	0.735881	7.781136	-0.000624	-0.158666	-0.158978
2	5	0.215614	-0.767014	9.516283	0.005299	0.165379	0.168028
3	4	-1.239831	0.735881	3.590480	0.070770	0.912368	0.947753
3	5	-1.239831	-0.767014	5.325626	0.046513	-0.950968	-0.927711
4	5	0.735881	-0.767014	1.735147	0.375913	0.564431	0.752388

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-159.00	-122.88	87.91	71.01	-71.09	-51.87
1	3	-334.28	-232.60	-633.66	-377.27	-967.94	-609.87
1	4	0.12	0.14	99.12	84.55	99.24	84.69
1	5	-0.52	-0.62	-84.62	-67.75	-85.14	-68.36
2	3	-5.19	-6.34	-52.79	-40.03	-57.98	-46.37
2	4	0.02	0.03	13.63	12.80	13.65	12.82
2	5	-0.15	-0.17	-12.36	-10.91	-12.50	-11.08
3	4	-11.13	-6.18	-129.85	-159.46	-140.98	-165.64
3	5	-5.41	-2.74	108.41	112.05	103.00	109.31
4	5	-82.47	-67.97	-215.79	-204.12	-298.26	-272.10

MOLECULE & CALCULATION = CH4 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	0.00000000
2	H	1.18599212	1.18599212	1.18599212
3	H	1.18599212	-1.18599212	-1.18599212
4	H	-1.18599212	1.18599212	-1.18599212
5	H	-1.18599212	-1.18599212	1.18599212

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.167874	-0.041750	2.054199	0.785206	0.007009	0.399612
1	3	0.167874	-0.041750	2.054199	0.785206	0.007009	0.399612
1	4	0.167874	-0.041750	2.054199	0.785206	0.007009	0.399612
1	5	0.167874	-0.041750	2.054199	0.785206	0.007009	0.399612
2	3	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559
2	4	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559
2	5	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559
3	4	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559
3	5	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559
4	5	-0.041750	-0.041750	3.354492	0.060604	-0.001743	0.028559

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-161.58	-119.93	22.07	-2.14	-139.51	-122.07
1	3	-161.58	-119.93	22.07	-2.14	-139.51	-122.07
1	4	-161.58	-119.93	22.07	-2.14	-139.51	-122.07
1	5	-161.58	-119.93	22.07	-2.14	-139.51	-122.07

2	3	-4.99	-5.67	0.78	0.33	-4.21	-5.34
2	4	-4.99	-5.67	0.78	0.33	-4.21	-5.34
2	5	-4.99	-5.67	0.78	0.33	-4.21	-5.34
3	4	-4.99	-5.67	0.78	0.33	-4.21	-5.34
3	5	-4.99	-5.67	0.78	0.33	-4.21	-5.34
4	5	-4.99	-5.67	0.78	0.33	-4.21	-5.34

MOLECULE & CALCULATION = H2CF+ CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	1.10988062
2	F	0.00000000	0.00000000	-1.19653012
3	H	0.00000000	1.83001078	2.05474368
4	H	0.00000000	-1.83001078	2.05474368

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.938096	-0.499038	2.306411	0.890703	0.468146	0.913497
1	3	0.938096	0.280372	2.059540	0.706105	-0.263016	0.090037
1	4	0.938096	0.280372	2.059540	0.706105	-0.263016	0.090037
2	3	-0.499038	0.280372	3.730914	0.074871	0.139916	0.177352
2	4	-0.499038	0.280372	3.730914	0.074871	0.139916	0.177352
3	4	0.280372	0.280372	3.660022	0.044225	-0.078608	-0.056496

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-192.06	-121.17	-288.84	-127.37	-480.90	-248.54
1	3	-147.08	-107.57	84.49	80.14	-62.59	-27.43
1	4	-147.08	-107.57	84.49	80.14	-62.59	-27.43
2	3	-6.21	-6.30	-32.53	-23.53	-38.74	-29.83
2	4	-6.21	-6.30	-32.53	-23.53	-38.74	-29.83
3	4	-3.05	-3.79	17.34	13.48	14.28	9.69

MOLECULE & CALCULATION = HCN CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	0.00000000	0.00000000	2.95931111
2	C	0.00000000	0.00000000	0.94864251
3	N	0.00000000	0.00000000	-1.23588089

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.189547	1.022910	2.010669	0.801050	-0.193890	0.206635
1	3	0.189547	-1.211968	4.195192	0.091093	0.229725	0.275271
2	3	1.022910	-1.211968	2.184523	1.644167	1.239734	2.061818

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-161.31	-125.00	81.95	60.51	-79.36	-64.49
1	3	-5.54	-6.81	-46.53	-34.36	-52.06	-41.17
2	3	-337.92	-236.15	-610.89	-356.12	-948.81	-592.26

MOLECULE & CALCULATION = ETHYLENE CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	1.26517164
2	C	0.00000000	0.00000000	-1.26517164
3	H	0.00000000	1.75536660	2.32833156
4	H	0.00000000	-1.75536660	2.32833156
5	H	0.00000000	1.75536660	-2.32833156
6	H	0.00000000	-1.75536660	-2.32833156

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.041173	0.041173	2.530343	1.262072	-0.001695	0.629341
1	3	0.041173	-0.020503	2.052223	0.803165	0.000844	0.402427
1	4	0.041173	-0.020503	2.052223	0.803165	0.000844	0.402427
1	5	0.041173	-0.020503	3.999322	0.058243	0.000844	0.029966
1	6	0.041173	-0.020503	3.999322	0.058243	0.000844	0.029966
2	3	0.041173	-0.020503	3.999322	0.058243	0.000844	0.029966
2	4	0.041173	-0.020503	3.999322	0.058243	0.000844	0.029966
2	5	0.041173	-0.020503	2.052223	0.803165	0.000844	0.402427
2	6	0.041173	-0.020503	2.052223	0.803165	0.000844	0.402427
3	4	-0.020503	-0.020503	3.510733	0.056423	-0.000420	0.027791
3	5	-0.020503	-0.020503	4.656663	0.026036	-0.000420	0.012598
3	6	-0.020503	-0.020503	5.831789	0.020513	-0.000420	0.009836
4	5	-0.020503	-0.020503	5.831789	0.020513	-0.000420	0.009836
4	6	-0.020503	-0.020503	4.656663	0.026036	-0.000420	0.012598
5	6	-0.020503	-0.020503	3.510733	0.056423	-0.000420	0.027791

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-264.27	-156.49	43.96	0.42	-220.31	-156.07
1	3	-164.59	-122.79	23.87	-0.26	-140.71	-123.05
1	4	-164.59	-122.79	23.87	-0.26	-140.71	-123.05
1	5	-4.77	-4.57	1.42	-0.13	-3.36	-4.70
1	6	-4.77	-4.57	1.42	-0.13	-3.36	-4.70

2	3	-4.77	-4.57	1.42	-0.13	-3.36	-4.70
2	4	-4.77	-4.57	1.42	-0.13	-3.36	-4.70
2	5	-164.59	-122.79	23.87	-0.26	-140.71	-123.05
2	6	-164.59	-122.79	23.87	-0.26	-140.71	-123.05
3	4	-4.15	-5.04	0.72	0.08	-3.43	-4.97
3	5	-1.70	-1.75	0.22	0.06	-1.48	-1.70
3	6	-0.88	-1.10	0.08	0.05	-0.79	-1.06
4	5	-0.88	-1.10	0.08	0.05	-0.79	-1.06
4	6	-1.70	-1.75	0.22	0.06	-1.48	-1.70
5	6	-4.15	-5.04	0.72	0.08	-3.43	-4.97

MOLECULE & CALCULATION = HF_HF CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	F	0.17048607	-2.50146229	0.00000000
2	H	-1.38575291	-3.28899805	0.00000000
3	F	-0.03639156	2.75366476	0.00000000
4	H	0.17890229	1.01917587	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-0.717978	0.730242	1.744159	0.434528	0.524298	0.741562
1	3	-0.717978	-0.745941	5.259198	0.040687	-0.535569	-0.515226
1	4	-0.717978	0.733920	3.520648	0.046240	0.526938	0.550058
2	3	0.730242	-0.745941	6.191490	0.005096	0.544717	0.547265
2	4	0.730242	0.733920	4.583504	-0.001235	-0.535939	-0.536557
3	4	-0.745941	0.733920	1.747800	0.397423	0.547461	0.746173

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-90.54	-78.17	-194.05	-188.63	-284.59	-266.80
1	3	-4.10	-2.43	67.28	63.90	63.18	61.48
1	4	-7.37	-4.12	-84.70	-93.92	-92.07	-98.04
2	3	-0.21	-0.26	-60.75	-55.21	-60.96	-55.47
2	4	0.07	0.08	73.14	73.37	73.21	73.46
3	4	-85.99	-71.34	-205.70	-196.55	-291.70	-267.90

MOLECULE & CALCULATION = H2O CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	O	0.00000000	0.00000000	0.22166487
2	H	1.43090062	0.00000000	-0.88665950
3	H	-1.43090062	0.00000000	-0.88665950

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.170623	0.585182	1.809934	0.588630	0.685028	0.979343
1	3	-1.170623	0.585168	1.809934	0.588592	0.685011	0.979307
2	3	0.585182	0.585168	2.861801	0.021208	-0.342430	-0.331826

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-120.32	-102.04	-214.20	-237.50	-334.51	-339.54
1	3	-120.32	-102.03	-214.18	-237.50	-334.50	-339.53
2	3	-1.71	-2.33	87.78	75.08	86.07	72.76

MOLECULE & CALCULATION = CH4_HF CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	-2.95401043	0.00000000
2	H	0.00000000	-5.01003245	0.00000000
3	H	-1.93848106	-2.26860676	0.00000000
4	H	0.96924053	-2.26860676	-1.67864372
5	H	0.96924053	-2.26860676	1.67864372
6	F	0.00000000	3.12750618	0.00000000
7	H	0.00000000	1.39235966	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.142972	-0.014021	2.056022	0.780041	0.002005	0.392025
1	3	0.142972	-0.038085	2.056085	0.781502	0.005445	0.396196
1	4	0.142972	-0.038103	2.055979	0.781408	0.005448	0.396152
1	5	0.142972	-0.038103	2.055979	0.781408	0.005448	0.396152
1	6	0.142972	-0.724895	6.081517	0.007969	0.103640	0.107624
1	7	0.142972	0.711232	4.346370	0.019443	-0.101686	-0.091965
2	3	-0.014021	-0.038085	3.357547	0.057239	-0.000534	0.028086
2	4	-0.014021	-0.038103	3.357482	0.057237	-0.000534	0.028084
2	5	-0.014021	-0.038103	3.357482	0.057237	-0.000534	0.028084
2	6	-0.014021	-0.724895	8.137539	0.009966	-0.010164	-0.005181
2	7	-0.014021	0.711232	6.402392	-0.000815	0.009972	0.009565
3	4	-0.038085	-0.038103	3.357483	0.058816	-0.001451	0.027957
3	5	-0.038085	-0.038103	3.357483	0.058816	-0.001451	0.027957
3	6	-0.038085	-0.724895	5.733737	0.008092	-0.027608	-0.023562
3	7	-0.038085	0.711232	4.142509	0.007058	0.027087	0.030616
4	5	-0.038103	-0.038103	3.357287	0.058826	-0.001452	0.027961
4	6	-0.038103	-0.724895	5.733699	0.008088	-0.027621	-0.023577
4	7	-0.038103	0.711232	4.142457	0.007052	0.027100	0.030626
5	6	-0.038103	-0.724895	5.733699	0.008088	-0.027621	-0.023577
5	7	-0.038103	0.711232	4.142457	0.007052	0.027100	0.030626
6	7	-0.724895	0.711232	1.735147	0.432416	0.515569	0.731777

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-160.62	-119.04	23.70	-0.61	-136.92	-119.65
1	3	-161.42	-119.26	21.78	-1.66	-139.64	-120.92
1	4	-161.40	-119.25	21.79	-1.66	-139.61	-120.91
1	5	-161.40	-119.25	21.79	-1.66	-139.61	-120.91
1	6	-1.00	-0.41	-10.88	-10.69	-11.88	-11.11
1	7	-2.93	-1.40	12.19	14.68	9.26	13.28
2	3	-4.76	-5.35	0.76	0.10	-4.00	-5.25
2	4	-4.76	-5.35	0.75	0.10	-4.00	-5.25
2	5	-4.76	-5.35	0.75	0.10	-4.00	-5.25
2	6	-0.33	-0.38	-0.39	0.78	-0.71	0.40
2	7	0.02	0.04	0.71	-0.98	0.72	-0.94
3	4	-4.86	-5.50	0.74	0.27	-4.12	-5.23
3	5	-4.86	-5.50	0.74	0.27	-4.12	-5.23
3	6	-0.72	-0.44	3.54	3.02	2.82	2.58
3	7	-0.96	-0.53	-4.07	-4.10	-5.03	-4.64
4	5	-4.86	-5.50	0.74	0.27	-4.13	-5.23
4	6	-0.72	-0.44	3.54	3.02	2.82	2.58
4	7	-0.96	-0.53	-4.07	-4.11	-5.03	-4.64
5	6	-0.72	-0.44	3.54	3.02	2.82	2.58
5	7	-0.96	-0.53	-4.07	-4.11	-5.03	-4.64
6	7	-92.18	-78.19	-192.75	-186.45	-284.93	-264.64

MOLECULE & CALCULATION = CH4_CH4 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00008902	3.51337881	0.00000000
2	C	-0.00008902	-3.51337881	0.00000000
3	H	-0.00042575	5.57147955	0.00000000
4	H	0.00042575	-5.57147955	0.00000000
5	H	-0.96973588	2.82440924	1.67902166
6	H	0.96973588	-2.82440924	-1.67902166
7	H	-0.96973588	2.82440924	-1.67902166
8	H	0.96973588	-2.82440924	1.67902166
9	H	1.93930853	2.82490245	0.00000000
10	H	-1.93930853	-2.82490245	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.166620	0.166620	7.026758	0.004402	-0.027762	-0.025561
1	3	0.166620	-0.042359	2.058101	0.783754	0.007058	0.398935
1	4	0.166620	-0.042359	9.084858	-0.000446	0.007058	0.006835
1	5	0.166620	-0.041361	2.057754	0.781949	0.006892	0.397866
1	6	0.166620	-0.041361	6.627736	0.002549	0.006892	0.008166
1	7	0.166620	-0.041361	2.057754	0.781949	0.006892	0.397866
1	8	0.166620	-0.041361	6.627736	0.002549	0.006892	0.008166
1	9	0.166620	-0.041369	2.057808	0.782177	0.006893	0.397981
1	10	0.166620	-0.041369	6.628354	0.002536	0.006893	0.008161
2	3	0.166620	-0.042359	9.084858	-0.000446	0.007058	0.006835

2	4	0.166620	-0.042359	2.058101	0.783754	0.007058	0.398935
2	5	0.166620	-0.041361	6.627736	0.002549	0.006892	0.008166
2	6	0.166620	-0.041361	2.057754	0.781949	0.006892	0.397866
2	7	0.166620	-0.041361	6.627736	0.002549	0.006892	0.008166
2	8	0.166620	-0.041361	2.057754	0.781949	0.006892	0.397866
2	9	0.166620	-0.041369	6.628354	0.002536	0.006893	0.008161
2	10	0.166620	-0.041369	2.057808	0.782177	0.006893	0.397981
3	4	-0.042359	-0.042359	11.142959	0.004408	-0.001794	0.000410
3	5	-0.042359	-0.041361	3.362301	0.059778	-0.001752	0.028137
3	6	-0.042359	-0.041361	8.616918	-0.000060	-0.001752	-0.001782
3	7	-0.042359	-0.041361	3.362301	0.059778	-0.001752	0.028137
3	8	-0.042359	-0.041361	8.616918	-0.000060	-0.001752	-0.001782
3	9	-0.042359	-0.041369	3.362477	0.059775	-0.001752	0.028135
3	10	-0.042359	-0.041369	8.617337	-0.000057	-0.001752	-0.001781
4	5	-0.042359	-0.041361	8.616918	-0.000060	-0.001752	-0.001782
4	6	-0.042359	-0.041361	3.362301	0.059778	-0.001752	0.028137
4	7	-0.042359	-0.041361	8.616918	-0.000060	-0.001752	-0.001782
4	8	-0.042359	-0.041361	3.362301	0.059778	-0.001752	0.028137
4	9	-0.042359	-0.041369	8.617337	-0.000057	-0.001752	-0.001781
4	10	-0.042359	-0.041369	3.362477	0.059775	-0.001752	0.028135
5	6	-0.041361	-0.041361	6.851799	-0.004189	-0.001711	-0.003805
5	7	-0.041361	-0.041361	3.358043	0.059491	-0.001711	0.028035
5	8	-0.041361	-0.041361	5.972495	0.005864	-0.001711	0.001221
5	9	-0.041361	-0.041369	3.358817	0.059461	-0.001711	0.028019
5	10	-0.041361	-0.041369	5.972764	0.005865	-0.001711	0.001221
6	7	-0.041361	-0.041361	5.972495	0.005864	-0.001711	0.001221
6	8	-0.041361	-0.041361	3.358043	0.059491	-0.001711	0.028035
6	9	-0.041361	-0.041369	5.972764	0.005865	-0.001711	0.001221
6	10	-0.041361	-0.041369	3.358817	0.059461	-0.001711	0.028019
7	8	-0.041361	-0.041361	6.851799	-0.004189	-0.001711	-0.003805
7	9	-0.041361	-0.041369	3.358817	0.059461	-0.001711	0.028019
7	10	-0.041361	-0.041369	5.972764	0.005865	-0.001711	0.001221
8	9	-0.041361	-0.041369	5.972764	0.005865	-0.001711	0.001221
8	10	-0.041361	-0.041369	3.358817	0.059461	-0.001711	0.028019
9	10	-0.041369	-0.041369	6.853026	-0.004188	-0.001711	-0.003805

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-0.51	-0.20	2.34	2.48	1.83	2.28
1	3	-161.28	-119.48	21.81	-2.15	-139.46	-121.63
1	4	0.03	0.02	-0.31	-0.49	-0.28	-0.47
1	5	-161.08	-119.23	21.87	-2.10	-139.21	-121.33
1	6	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
1	7	-161.08	-119.23	21.87	-2.10	-139.21	-121.33
1	8	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
1	9	-161.13	-119.26	21.87	-2.10	-139.25	-121.36
1	10	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
2	3	0.03	0.02	-0.31	-0.49	-0.28	-0.47
2	4	-161.28	-119.48	21.81	-2.15	-139.46	-121.63
2	5	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
2	6	-161.08	-119.23	21.87	-2.10	-139.21	-121.33
2	7	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
2	8	-161.08	-119.23	21.87	-2.10	-139.21	-121.33
2	9	-0.27	-0.12	-0.71	-0.65	-0.98	-0.77
2	10	-161.13	-119.26	21.87	-2.10	-139.25	-121.36

3	4	-0.11	-0.12	0.06	0.10	-0.05	-0.02
3	5	-4.94	-5.58	0.77	0.33	-4.17	-5.25
3	6	0.00	0.00	0.08	0.13	0.08	0.13
3	7	-4.94	-5.58	0.77	0.33	-4.17	-5.25
3	8	0.00	0.00	0.08	0.13	0.08	0.13
3	9	-4.94	-5.58	0.77	0.33	-4.17	-5.25
3	10	0.00	0.00	0.08	0.13	0.08	0.13
4	5	0.00	0.00	0.08	0.13	0.08	0.13
4	6	-4.94	-5.58	0.77	0.33	-4.17	-5.25
4	7	0.00	0.00	0.08	0.13	0.08	0.13
4	8	-4.94	-5.58	0.77	0.33	-4.17	-5.25
4	9	0.00	0.00	0.08	0.13	0.08	0.13
4	10	-4.94	-5.58	0.77	0.33	-4.17	-5.25
5	6	0.17	0.19	0.08	0.16	0.25	0.35
5	7	-4.92	-5.56	0.77	0.32	-4.15	-5.24
5	8	-0.47	-0.31	0.26	0.18	-0.20	-0.13
5	9	-4.91	-5.55	0.77	0.32	-4.14	-5.23
5	10	-0.46	-0.31	0.26	0.18	-0.20	-0.13
6	7	-0.47	-0.31	0.26	0.18	-0.20	-0.13
6	8	-4.92	-5.56	0.77	0.32	-4.15	-5.24
6	9	-0.46	-0.31	0.26	0.18	-0.20	-0.13
6	10	-4.91	-5.55	0.77	0.32	-4.14	-5.23
7	8	0.17	0.19	0.08	0.16	0.25	0.35
7	9	-4.91	-5.55	0.77	0.32	-4.14	-5.23
7	10	-0.46	-0.31	0.26	0.18	-0.20	-0.13
8	9	-0.46	-0.31	0.26	0.18	-0.20	-0.13
8	10	-4.91	-5.55	0.77	0.32	-4.14	-5.23
9	10	0.17	0.19	0.08	0.16	0.25	0.35

MOLECULE & CALCULATION = H2O_H2O CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	O	-2.99064664	0.21868084	0.00000000
2	H	-3.69225240	-1.41878192	0.00000000
3	H	-1.21427527	-0.00784860	0.00000000
4	O	2.72458998	-0.17647995	0.00000000
5	H	3.51749047	0.54451173	1.42655425
6	H	3.51749047	0.54451173	-1.42655425

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.230569	0.585141	1.781442	0.592595	0.720056	1.016354
1	3	-1.230569	0.632006	1.790757	0.507224	0.777727	1.031339
1	4	-1.230569	-1.204372	5.728881	0.031394	-1.482063	-1.466366
1	5	-1.230569	0.608676	6.670613	0.004649	0.749018	0.751342
1	6	-1.230569	0.608676	6.670613	0.004649	0.749018	0.751342
2	3	0.585141	0.632006	2.851509	0.015622	-0.369813	-0.362002
2	4	0.585141	-1.204372	6.535991	0.001431	0.704727	0.705443
2	5	0.585141	0.608676	7.607232	0.001026	-0.356161	-0.355648
2	6	0.585141	0.608676	7.607232	0.001026	-0.356161	-0.355648
3	4	0.632006	-1.204372	3.942473	0.054243	0.761170	0.788292

3	5	0.632006	0.608676	4.972903	-0.001266	-0.384687	-0.385320
3	6	0.632006	0.608676	4.972903	-0.001266	-0.384687	-0.385320
4	5	-1.204372	0.608676	1.784258	0.563851	0.733072	1.014998
4	6	-1.204372	0.608676	1.784258	0.563851	0.733072	1.014998
5	6	0.608676	0.608676	2.853108	0.018533	-0.370486	-0.361220

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-122.26	-104.37	-222.74	-253.64	-345.00	-358.01
1	3	-108.87	-88.87	-248.14	-272.53	-357.01	-361.40
1	4	-3.12	-1.72	160.72	162.34	157.59	160.62
1	5	-0.19	-0.22	-73.36	-70.46	-73.55	-70.68
1	6	-0.19	-0.22	-73.36	-70.46	-73.55	-70.68
2	3	-1.30	-1.72	93.88	81.38	92.58	79.66
2	4	-0.06	-0.07	-67.25	-67.66	-67.30	-67.73
2	5	-0.04	-0.04	30.83	29.38	30.80	29.34
2	6	-0.04	-0.04	30.83	29.38	30.80	29.34
3	4	-7.87	-4.32	-110.38	-121.15	-118.25	-125.47
3	5	0.06	0.08	48.32	48.54	48.38	48.62
3	6	0.06	0.08	48.32	48.54	48.38	48.62
4	5	-117.04	-99.15	-229.12	-257.82	-346.16	-356.97
4	6	-117.04	-99.15	-229.12	-257.82	-346.16	-356.97
5	6	-1.48	-2.04	94.18	81.48	92.70	79.45

MOLECULE & CALCULATION = OC_BH3 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	-0.00001022	0.00004855	-0.42362579
2	B	0.00000170	-0.00001590	2.63852689
3	H	1.45553127	1.68956642	3.15188207
4	H	-2.19093933	0.41566267	3.15200414
5	H	0.73550803	-2.10538160	3.15159043
6	O	-0.00000589	-0.00000742	-2.51329454

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	1.094737	1.921866	3.062153	0.308753	-2.103938	-1.949561
1	3	1.094737	-0.615495	4.213944	0.170869	0.673805	0.759240
1	4	1.094737	-0.615508	4.214028	0.170831	0.673819	0.759235
1	5	1.094737	-0.615447	4.213786	0.170847	0.673753	0.759176
1	6	1.094737	-1.169340	2.089669	1.220331	1.280120	1.890285
2	3	1.921866	-0.615495	2.288403	0.446098	1.182899	1.405948
2	4	1.921866	-0.615508	2.288377	0.446364	1.182924	1.406106
2	5	1.921866	-0.615447	2.288399	0.446636	1.182807	1.406125
2	6	1.921866	-1.169340	5.151821	0.004475	2.247315	2.249552
3	4	-0.615495	-0.615508	3.862587	0.117389	-0.378842	-0.320148
3	5	-0.615495	-0.615447	3.862650	0.117381	-0.378805	-0.320114
3	6	-0.615495	-1.169340	6.088306	0.044489	-0.719723	-0.697478
4	5	-0.615508	-0.615447	3.862610	0.117377	-0.378813	-0.320124

4	6	-0.615508	-1.169340	6.088397	0.044489	-0.719738	-0.697494
5	6	-0.615447	-1.169340	6.088062	0.044493	-0.719667	-0.697420

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-63.08	-31.64	201.64	431.15	138.57	399.51
1	3	-24.16	-12.72	-69.38	-100.34	-93.54	-113.06
1	4	-24.15	-12.72	-69.39	-100.34	-93.54	-113.06
1	5	-24.16	-12.72	-69.38	-100.33	-93.53	-113.06
1	6	-265.52	-183.23	-800.10	-384.41	-1065.62	-567.64
2	3	-89.28	-61.16	-360.05	-324.37	-449.33	-385.53
2	4	-89.34	-61.20	-360.01	-324.38	-449.35	-385.58
2	5	-89.40	-61.24	-359.93	-324.34	-449.32	-385.58
2	6	-0.25	-0.27	-321.17	-273.73	-321.42	-274.00
3	4	-14.27	-9.54	71.02	61.55	56.74	52.01
3	5	-14.27	-9.53	71.01	61.54	56.74	52.00
3	6	-2.22	-2.29	87.40	74.18	85.18	71.89
4	5	-14.27	-9.53	71.01	61.54	56.74	52.01
4	6	-2.22	-2.29	87.40	74.18	85.18	71.89
5	6	-2.22	-2.29	87.39	74.18	85.17	71.88

MOLECULE & CALCULATION = CH4_NH3 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000113	-3.76718793	0.00000000
2	H	-0.00000465	-1.71116590	0.00000000
3	H	1.93848411	-4.45258615	0.00000000
4	H	-0.96923748	-4.45259431	-1.67864372
5	H	-0.96923748	-4.45259431	1.67864372
6	N	-0.00001956	3.60274396	0.00000000
7	H	-1.83286647	4.15094836	0.00000000
8	H	0.91649607	4.15095608	1.58736994
9	H	0.91649607	4.15095608	-1.58736994

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.150254	0.002860	2.056022	0.774491	-0.000430	0.386816
1	3	0.150254	-0.053411	2.056085	0.787268	0.008025	0.401659
1	4	0.150254	-0.053549	2.055979	0.787416	0.008046	0.401754
1	5	0.150254	-0.053549	2.055979	0.787416	0.008046	0.401754
1	6	0.150254	-1.218900	7.369932	0.004603	0.183145	0.185446
1	7	0.150254	0.408886	8.127502	0.001166	-0.061437	-0.060854
1	8	0.150254	0.408876	8.127528	0.001166	-0.061435	-0.060852
1	9	0.150254	0.408876	8.127528	0.001166	-0.061435	-0.060852
2	3	0.002860	-0.053411	3.357547	0.056340	0.000153	0.028323
2	4	0.002860	-0.053549	3.357482	0.056356	0.000153	0.028331
2	5	0.002860	-0.053549	3.357482	0.056356	0.000153	0.028331
2	6	0.002860	-1.218900	5.313910	0.044411	0.003486	0.025692
2	7	0.002860	0.408886	6.141968	-0.001559	-0.001169	-0.001949

2	8	0.002860	0.408876	6.142002	-0.001559	-0.001169	-0.001949
2	9	0.002860	0.408876	6.142002	-0.001559	-0.001169	-0.001949
3	4	-0.053411	-0.053549	3.357483	0.061780	-0.002860	0.028030
3	5	-0.053411	-0.053549	3.357483	0.061780	-0.002860	0.028030
3	6	-0.053411	-1.218900	8.285297	-0.000603	-0.065103	-0.065404
3	7	-0.053411	0.408886	9.393822	-0.000233	0.021839	0.021723
3	8	-0.053411	0.408876	8.808243	0.001799	0.021838	0.022738
3	9	-0.053411	0.408876	8.808243	0.001799	0.021838	0.022738
4	5	-0.053549	-0.053549	3.357287	0.061788	-0.002867	0.028027
4	6	-0.053549	-1.218900	8.285270	-0.000602	-0.065271	-0.065572
4	7	-0.053549	0.408886	8.808215	0.001799	0.021895	0.022795
4	8	-0.053549	0.408876	9.393823	-0.000233	0.021895	0.021778
4	9	-0.053549	0.408876	8.808258	0.001799	0.021895	0.022794
5	6	-0.053549	-1.218900	8.285270	-0.000602	-0.065271	-0.065572
5	7	-0.053549	0.408886	8.808215	0.001799	0.021895	0.022795
5	8	-0.053549	0.408876	8.808258	0.001799	0.021895	0.022794
5	9	-0.053549	0.408876	9.393823	-0.000233	0.021895	0.021778
6	7	-1.218900	0.408886	1.913075	0.705173	0.498391	0.850978
6	8	-1.218900	0.408876	1.913186	0.705212	0.498379	0.850985
6	9	-1.218900	0.408876	1.913186	0.705212	0.498379	0.850985
7	8	0.408886	0.408876	3.174703	0.030347	-0.167184	-0.152010
7	9	0.408886	0.408876	3.174703	0.030347	-0.167184	-0.152010
8	9	0.408876	0.408876	3.174740	0.030347	-0.167180	-0.152006

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-160.44	-118.19	24.39	0.13	-136.05	-118.06
1	3	-161.74	-120.14	21.20	-2.45	-140.54	-122.58
1	4	-161.79	-120.16	21.19	-2.46	-140.60	-122.62
1	5	-161.79	-120.16	21.19	-2.46	-140.60	-122.62
1	6	-0.35	-0.20	-16.00	-15.59	-16.35	-15.79
1	7	-0.05	-0.05	4.86	4.74	4.81	4.70
1	8	-0.05	-0.05	4.86	4.74	4.81	4.70
1	9	-0.05	-0.05	4.86	4.74	4.81	4.70
2	3	-4.70	-5.26	0.68	-0.03	-4.02	-5.29
2	4	-4.70	-5.27	0.68	-0.03	-4.02	-5.30
2	5	-4.70	-5.27	0.68	-0.03	-4.02	-5.30
2	6	-4.81	-2.62	1.20	-0.41	-3.61	-3.03
2	7	0.05	0.08	-0.38	0.12	-0.32	0.20
2	8	0.05	0.08	-0.38	0.12	-0.32	0.20
2	9	0.05	0.08	-0.38	0.12	-0.32	0.20
3	4	-5.09	-5.77	0.81	0.53	-4.28	-5.24
3	5	-5.09	-5.77	0.81	0.53	-4.28	-5.24
3	6	0.02	0.02	4.13	4.93	4.15	4.95
3	7	0.01	0.01	-1.21	-1.46	-1.20	-1.45
3	8	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62
3	9	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62
4	5	-5.09	-5.77	0.81	0.54	-4.28	-5.24
4	6	0.02	0.02	4.14	4.94	4.16	4.97
4	7	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62
4	8	0.01	0.01	-1.22	-1.46	-1.21	-1.45
4	9	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62
5	6	0.02	0.02	4.14	4.94	4.16	4.97
5	7	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62
5	8	-0.06	-0.06	-1.38	-1.56	-1.44	-1.62

5	9	0.01	0.01	-1.22	-1.46	-1.21	-1.45
6	7	-143.18	-115.65	-131.44	-163.48	-274.63	-279.13
6	8	-143.20	-115.65	-131.51	-163.46	-274.72	-279.12
6	9	-143.20	-115.65	-131.51	-163.46	-274.72	-279.12
7	8	-2.21	-3.00	43.16	33.05	40.95	30.05
7	9	-2.21	-3.00	43.16	33.05	40.95	30.05
8	9	-2.21	-3.00	43.16	33.04	40.95	30.05

MOLECULE & CALCULATION = HF_N2 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	0.00000000	0.00000000	-2.38147066
2	F	0.00000000	0.00000000	-4.08706187
3	N	0.00000000	0.00000000	1.84029089
4	N	0.00000000	0.00000000	3.87450547

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.729900	-0.740317	1.705591	0.413764	0.540357	0.747239
1	3	0.729900	-0.032335	4.221762	0.038404	0.023601	0.042803
1	4	0.729900	0.042560	6.255976	-0.005027	-0.031065	-0.033578
2	3	-0.740317	-0.032335	5.927353	0.014453	-0.023938	-0.016712
2	4	-0.740317	0.042560	7.961567	0.015243	0.031508	0.039129
3	4	-0.032335	0.042560	2.034215	1.988360	0.001376	0.995556

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-89.41	-76.11	-204.99	-198.80	-294.41	-274.92
1	3	-5.18	-2.85	-15.99	-3.51	-21.17	-6.36
1	4	0.23	0.25	11.55	3.12	11.77	3.37
2	3	-1.96	-0.77	11.39	2.53	9.42	1.77
2	4	-0.49	-0.60	-8.90	-2.48	-9.39	-3.08
3	4	-449.32	-306.68	162.95	-0.42	-286.37	-307.11

MOLECULE & CALCULATION = CH2O_CH2O CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	-0.92686005	3.27835406	0.00000000
2	C	0.95443403	-2.90204366	0.00000000
3	O	-1.27537624	-3.15697359	0.00000000
4	H	2.04447532	-2.78353318	-1.76009091

5	H	2.04447532	-2.78353318	1.76009091
6	O	1.23638456	2.67743446	0.00000000
7	H	-1.49411981	5.27483426	0.00000000
8	H	-2.44834129	1.87068280	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	1.172570	1.204352	6.460386	0.000121	-1.412187	-1.412127
1	3	1.172570	-1.125136	6.444758	0.008610	1.319301	1.323606
1	4	1.172570	-0.040261	6.976620	0.000552	0.047209	0.047485
1	5	1.172570	-0.040261	6.976620	0.000552	0.047209	0.047485
1	6	1.172570	-1.118196	2.245157	1.116229	1.311163	1.869278
1	7	1.172570	-0.037933	2.075504	0.744880	0.044479	0.416919
1	8	1.172570	-0.014998	2.072786	0.740594	0.017586	0.387883
2	3	1.204352	-1.125136	2.244336	1.102258	1.355060	1.906189
2	4	1.204352	-0.040261	2.073681	0.738661	0.048488	0.417819
2	5	1.204352	-0.040261	2.073681	0.738661	0.048488	0.417819
2	6	1.204352	-1.118196	5.586598	0.036709	1.346702	1.365056
2	7	1.204352	-0.037933	8.535616	-0.000773	0.045685	0.045298
2	8	1.204352	-0.014998	5.861553	-0.001780	0.018063	0.017173
3	4	-1.125136	-0.040261	3.776082	0.119401	-0.045299	0.014401
3	5	-1.125136	-0.040261	3.776082	0.119401	-0.045299	0.014401
3	6	-1.125136	-1.118196	6.352107	0.005335	-1.258123	-1.255455
3	7	-1.125136	-0.037933	8.434645	0.002532	-0.042680	-0.041414
3	8	-1.125136	-0.014998	5.162671	0.033745	-0.016875	-0.000002
4	5	-0.040261	-0.040261	3.520182	0.072431	-0.001621	0.034595
4	6	-0.040261	-1.118196	5.794230	0.011761	-0.045020	-0.039139
4	7	-0.040261	-0.037933	8.975347	0.002031	-0.001527	-0.000512
4	8	-0.040261	-0.014998	6.704107	-0.002765	-0.000604	-0.001986
5	6	-0.040261	-1.118196	5.794230	0.011761	-0.045020	-0.039139
5	7	-0.040261	-0.037933	8.975347	0.002031	-0.001527	-0.000512
5	8	-0.040261	-0.014998	6.704107	-0.002765	-0.000604	-0.001986
6	7	-1.118196	-0.037933	3.768573	0.119952	-0.042417	0.017559
6	8	-1.118196	-0.014998	3.772009	0.113830	-0.016771	0.040144
7	8	-0.037933	-0.014998	3.535362	0.069241	-0.000569	0.034052

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-0.09	-0.01	145.71	137.17	145.62	137.16
1	3	-0.67	-0.42	-134.27	-128.46	-134.94	-128.88
1	4	-0.03	-0.02	-3.81	-4.25	-3.84	-4.27
1	5	-0.03	-0.02	-3.81	-4.25	-3.84	-4.27
1	6	-245.09	-155.99	-595.64	-366.46	-840.74	-522.45
1	7	-155.52	-112.60	24.19	-13.45	-131.34	-126.05
1	8	-155.38	-112.10	30.57	-5.32	-124.81	-117.43
2	3	-244.07	-154.09	-608.49	-378.87	-852.57	-532.97
2	4	-155.07	-111.76	23.56	-14.67	-131.51	-126.43
2	5	-155.07	-111.76	23.56	-14.67	-131.51	-126.43
2	6	-4.38	-2.06	-146.43	-151.27	-150.81	-153.33
2	7	0.05	0.03	-1.80	-3.36	-1.75	-3.33
2	8	-0.01	0.10	-2.39	-1.93	-2.40	-1.84
3	4	-10.36	-9.92	-0.68	7.53	-11.04	-2.39
3	5	-10.36	-9.92	-0.68	7.53	-11.04	-2.39

3	6	-1.05	-0.26	131.30	124.29	130.25	124.02
3	7	-0.07	-0.09	1.71	3.18	1.64	3.08
3	8	-3.39	-2.05	2.73	2.05	-0.66	0.00
4	5	-5.10	-6.46	0.62	0.29	-4.48	-6.17
4	6	-1.05	-0.64	4.08	4.88	3.03	4.24
4	7	-0.06	-0.07	0.06	0.11	0.00	0.04
4	8	0.11	0.13	0.02	0.06	0.13	0.19
5	6	-1.05	-0.64	4.08	4.88	3.03	4.24
5	7	-0.06	-0.07	0.06	0.11	0.00	0.04
5	8	0.11	0.13	0.02	0.06	0.13	0.19
6	7	-10.46	-9.99	-1.18	7.06	-11.64	-2.92
6	8	-9.89	-9.47	-5.68	2.79	-15.56	-6.68
7	8	-4.91	-6.14	0.62	0.10	-4.30	-6.04

MOLECULE & CALCULATION = FORMIC CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.75436906	0.24609596	0.00000000
2	O	-0.12244944	-2.13562145	0.00000000
3	O	-0.54481544	2.10936070	0.00000000
4	H	2.76679644	0.74378470	0.00000000
5	H	-1.95489179	-2.01027452	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	1.642104	-1.141931	2.537989	0.753375	1.875169	2.251857
1	3	1.642104	-1.170172	2.271483	1.014708	1.921544	2.428898
1	4	1.642104	0.047941	2.073055	0.719792	-0.078724	0.281172
1	5	1.642104	0.622392	3.525805	0.006424	-1.022032	-1.018820
2	3	-1.141931	-1.170172	4.265943	0.218351	-1.336256	-1.227080
2	4	-1.141931	0.047941	4.079059	0.069765	0.054745	0.089628
2	5	-1.141931	0.622392	1.836724	0.513646	0.710729	0.967552
3	4	-1.170172	0.047941	3.582118	0.123800	0.056099	0.117999
3	5	-1.170172	0.622392	4.354275	0.037997	0.728306	0.747304
4	5	0.047941	0.622392	5.466185	0.013819	-0.029838	-0.022929

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-168.22	-93.13	-525.46	-463.63	-693.68	-556.76
1	3	-229.63	-140.16	-725.18	-530.84	-954.82	-671.00
1	4	-151.19	-108.94	59.27	23.83	-91.92	-85.11
1	5	-0.70	-0.57	211.54	181.90	210.84	181.33
2	3	-24.21	-16.06	223.33	196.56	199.12	180.50
2	4	-5.37	-5.37	-13.42	-8.42	-18.79	-13.79
2	5	-107.57	-87.74	-226.75	-242.82	-334.33	-330.56
3	4	-12.28	-10.84	-21.06	-9.83	-33.34	-20.67
3	5	-3.14	-2.74	-114.68	-104.96	-117.82	-107.70
4	5	-0.64	-0.79	5.48	3.43	4.84	2.63

MOLECULE & CALCULATION = HF_H2O CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	-0.78996763	0.08008580	0.00000000
2	F	-2.51240547	0.00832995	0.00000000
3	O	2.59619819	0.00674352	0.00000000
4	H	3.44683368	-0.65970917	1.42724168
5	H	3.44683368	-0.65970917	-1.42724168

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.748933	-0.779498	1.723932	0.356787	0.583792	0.762185
1	3	0.748933	-1.202329	3.386960	0.069763	0.900464	0.935345
1	4	0.748933	0.616767	4.531534	-0.000378	-0.461917	-0.462106
1	5	0.748933	0.616767	4.531534	-0.000378	-0.461917	-0.462106
2	3	-0.779498	-1.202329	5.108604	0.059901	-0.937213	-0.907263
2	4	-0.779498	0.616767	6.164075	0.007027	0.480769	0.484282
2	5	-0.779498	0.616767	6.164075	0.007027	0.480769	0.484282
3	4	-1.202329	0.616767	1.790184	0.552975	0.741557	1.018044
3	5	-1.202329	0.616767	1.790184	0.552975	0.741557	1.018044
4	5	0.616767	0.616767	2.854483	0.017868	-0.380402	-0.371468

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-79.36	-64.94	-224.17	-212.50	-303.53	-277.43
1	3	-11.59	-6.46	-149.68	-166.83	-161.27	-173.29
1	4	0.01	0.03	64.96	63.96	64.97	63.99
1	5	0.01	0.03	64.96	63.96	64.97	63.99
2	3	-6.62	-3.68	120.74	115.12	114.12	111.44
2	4	-0.30	-0.36	-54.66	-48.94	-54.96	-49.30
2	5	-0.30	-0.36	-54.66	-48.94	-54.96	-49.30
3	4	-114.89	-96.92	-233.14	-259.94	-348.03	-356.85
3	5	-114.89	-96.92	-233.14	-259.94	-348.03	-356.85
4	5	-1.43	-1.96	96.09	83.62	94.65	81.66

MOLECULE & CALCULATION = HF_F2 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	H	-2.55993639	0.20528095	0.00000000
2	F	-4.20484850	-0.23889918	0.00000000
3	F	1.48472002	1.18712595	0.00000000
4	F	2.85592419	-0.95911160	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.726761	-0.730467	1.703829	0.429393	0.530875	0.745571
1	3	0.726761	-0.013111	4.162123	0.021589	0.009529	0.020323
1	4	0.726761	0.016829	5.539617	-0.002173	-0.012231	-0.013317
2	3	-0.730467	-0.013111	5.865555	0.011545	-0.009577	-0.003805
2	4	-0.730467	0.016829	7.097409	0.006666	0.012293	0.015626
3	4	-0.013111	0.016829	2.546868	0.925247	0.000221	0.462844

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-92.47	-79.07	-198.29	-195.52	-290.76	-274.59
1	3	-2.89	-1.63	-5.86	-1.44	-8.75	-3.06
1	4	0.07	0.12	4.45	1.39	4.53	1.51
2	3	-1.30	-0.62	3.79	1.02	2.49	0.41
2	4	-0.27	-0.29	-3.05	-1.09	-3.32	-1.38
3	4	-172.48	-113.98	48.60	-0.05	-123.88	-114.04

MOLECULE & CALCULATION = NH3_F2 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	N	-4.06295841	-0.00001846	0.00000000
2	H	-4.78937425	1.77575509	0.00000000
3	H	-4.78936658	-0.88781388	1.53785912
4	H	-4.78936658	-0.88781388	-1.53785912
5	F	1.03136528	-0.00000378	0.00000000
6	F	3.72516987	0.00000398	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.140102	0.387498	1.918607	0.713488	0.441787	0.798531
1	3	-1.140102	0.387467	1.918557	0.713617	0.441752	0.798560
1	4	-1.140102	0.387467	1.918557	0.713617	0.441752	0.798560
1	5	-1.140102	0.006295	5.094324	0.075333	0.007177	0.044843
1	6	-1.140102	-0.028054	7.788128	-0.001535	-0.031984	-0.032752
2	3	0.387498	0.387467	3.075648	0.032409	-0.150143	-0.133938
2	4	0.387498	0.387467	3.075648	0.032409	-0.150143	-0.133938
2	5	0.387498	0.006295	6.085584	-0.000098	-0.002439	-0.002488
2	6	0.387498	-0.028054	8.697744	0.005087	0.010871	0.013414
3	4	0.387467	0.387467	3.075718	0.032410	-0.150131	-0.133926
3	5	0.387467	0.006295	6.085568	-0.000098	-0.002439	-0.002488
3	6	0.387467	-0.028054	8.697733	0.005087	0.010870	0.013413
4	5	0.387467	0.006295	6.085568	-0.000098	-0.002439	-0.002488
4	6	0.387467	-0.028054	8.697733	0.005087	0.010870	0.013413
5	6	0.006295	-0.028054	2.693805	0.827886	0.000177	0.414120

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-144.76	-116.68	-117.85	-144.49	-262.61	-261.17
1	3	-144.81	-116.70	-117.94	-144.49	-262.75	-261.19
1	4	-144.81	-116.70	-117.94	-144.49	-262.75	-261.19
1	5	-9.25	-4.64	0.12	-0.88	-9.13	-5.52
1	6	0.10	0.06	-1.46	2.58	-1.37	2.64
2	3	-2.49	-3.31	40.98	30.63	38.49	27.33
2	4	-2.49	-3.31	40.98	30.63	38.49	27.33
2	5	-0.02	0.01	-0.22	0.25	-0.24	0.26
2	6	-0.17	-0.18	0.29	-0.78	0.12	-0.97
3	4	-2.49	-3.31	40.97	30.63	38.49	27.32
3	5	-0.02	0.01	-0.22	0.25	-0.24	0.26
3	6	-0.17	-0.18	0.29	-0.78	0.12	-0.97
4	5	-0.02	0.01	-0.22	0.25	-0.24	0.26
4	6	-0.17	-0.18	0.29	-0.78	0.12	-0.97
5	6	-145.55	-96.43	33.26	-0.04	-112.29	-96.47

MOLECULE & CALCULATION = CH3F_CH3F CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	1.01825528	-3.54155605	0.00000000
2	C	-1.01825528	3.54155605	0.00000000
3	H	2.16766337	-1.83477721	0.00000000
4	H	-2.16766337	1.83477721	0.00000000
5	F	-1.50393048	-2.85644211	0.00000000
6	F	1.50393048	2.85644211	0.00000000
7	H	1.40151722	-4.65516398	1.68733646
8	H	-1.40151722	4.65516398	-1.68733646
9	H	1.40151722	-4.65516398	-1.68733646
10	H	-1.40151722	4.65516398	1.68733646

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.664367	0.664367	7.370065	0.000687	-0.441384	-0.441040
1	3	0.664367	0.007775	2.057725	0.741114	-0.005165	0.365392
1	4	0.664367	0.007775	6.249403	0.001420	-0.005165	-0.004455
1	5	0.664367	-0.611705	2.613580	0.671661	0.406397	0.742227
1	6	0.664367	-0.611705	6.416406	0.004777	0.406397	0.408785
1	7	0.664367	-0.030150	2.057697	0.749071	0.020031	0.394566
1	8	0.664367	-0.030150	8.711408	0.000293	0.020031	0.020177
1	9	0.664367	-0.030150	2.057697	0.749071	0.020031	0.394566
1	10	0.664367	-0.030150	8.711408	0.000293	0.020031	0.020177
2	3	0.664367	0.007775	6.249403	0.001420	-0.005165	-0.004455
2	4	0.664367	0.007775	2.057725	0.741114	-0.005165	0.365392
2	5	0.664367	-0.611705	6.416406	0.004777	0.406397	0.408785
2	6	0.664367	-0.611705	2.613580	0.671661	0.406397	0.742227
2	7	0.664367	-0.030150	8.711408	0.000293	0.020031	0.020177
2	8	0.664367	-0.030150	2.057697	0.749071	0.020031	0.394566
2	9	0.664367	-0.030150	8.711408	0.000293	0.020031	0.020177
2	10	0.664367	-0.030150	2.057697	0.749071	0.020031	0.394566

3	4	0.007775	0.007775	5.679849	-0.002808	-0.000060	-0.001464
3	5	0.007775	-0.611705	3.811089	0.073064	0.004756	0.041288
3	6	0.007775	-0.611705	4.737940	0.033322	0.004756	0.021417
3	7	0.007775	-0.030150	3.374710	0.055611	0.000234	0.028040
3	8	0.007775	-0.030150	7.596413	-0.001772	0.000234	-0.000652
3	9	0.007775	-0.030150	3.374710	0.055611	0.000234	0.028040
3	10	0.007775	-0.030150	7.596413	-0.001772	0.000234	-0.000652
4	5	0.007775	-0.611705	4.737940	0.033322	0.004756	0.021417
4	6	0.007775	-0.611705	3.811089	0.073064	0.004756	0.041288
4	7	0.007775	-0.030150	7.596413	-0.001772	0.000234	-0.000652
4	8	0.007775	-0.030150	3.374710	0.055611	0.000234	0.028040
4	9	0.007775	-0.030150	7.596413	-0.001772	0.000234	-0.000652
4	10	0.007775	-0.030150	3.374710	0.055611	0.000234	0.028040
5	6	-0.611705	-0.611705	6.456336	0.000107	-0.374183	-0.374130
5	7	-0.611705	-0.030150	3.811054	0.078589	-0.018443	0.020852
5	8	-0.611705	-0.030150	7.699469	0.000557	-0.018443	-0.018164
5	9	-0.611705	-0.030150	3.811054	0.078589	-0.018443	0.020852
5	10	-0.611705	-0.030150	7.699469	0.000557	-0.018443	-0.018164
6	7	-0.611705	-0.030150	7.699469	0.000557	-0.018443	-0.018164
6	8	-0.611705	-0.030150	3.811054	0.078589	-0.018443	0.020852
6	9	-0.611705	-0.030150	7.699469	0.000557	-0.018443	-0.018164
6	10	-0.611705	-0.030150	3.811054	0.078589	-0.018443	0.020852
7	8	-0.030150	-0.030150	10.292115	0.001288	-0.000909	-0.000265
7	9	-0.030150	-0.030150	3.374673	0.059322	-0.000909	0.028752
7	10	-0.030150	-0.030150	9.723128	0.002977	-0.000909	0.000579
8	9	-0.030150	-0.030150	9.723128	0.002977	-0.000909	0.000579
8	10	-0.030150	-0.030150	3.374673	0.059322	-0.000909	0.028752
9	10	-0.030150	-0.030150	10.292115	0.001288	-0.000909	-0.000265

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-0.06	-0.03	41.17	37.58	41.12	37.55
1	3	-157.22	-113.00	29.12	1.58	-128.10	-111.43
1	4	-0.13	-0.07	0.18	0.52	0.05	0.45
1	5	-145.94	-80.63	-147.16	-97.57	-293.10	-178.21
1	6	-0.44	-0.23	-40.67	-39.74	-41.11	-39.98
1	7	-157.89	-114.22	23.34	-6.11	-134.55	-120.33
1	8	-0.01	-0.01	-0.90	-1.44	-0.90	-1.45
1	9	-157.89	-114.22	23.34	-6.11	-134.55	-120.33
1	10	-0.01	-0.01	-0.90	-1.44	-0.90	-1.45
2	3	-0.13	-0.07	0.18	0.52	0.05	0.45
2	4	-157.22	-113.00	29.12	1.58	-128.10	-111.43
2	5	-0.44	-0.23	-40.67	-39.74	-41.11	-39.98
2	6	-145.94	-80.63	-147.16	-97.57	-293.10	-178.21
2	7	-0.01	-0.01	-0.90	-1.44	-0.90	-1.45
2	8	-157.89	-114.22	23.34	-6.11	-134.55	-120.33
2	9	-0.01	-0.01	-0.90	-1.44	-0.90	-1.45
2	10	-157.89	-114.22	23.34	-6.11	-134.55	-120.33
3	4	0.08	0.16	-0.02	0.01	0.06	0.16
3	5	-6.69	-6.02	-3.90	-0.78	-10.59	-6.80
3	6	-3.77	-2.21	-0.05	-0.63	-3.82	-2.84
3	7	-4.55	-5.17	0.74	-0.04	-3.81	-5.21
3	8	0.07	0.07	-0.01	-0.02	0.06	0.05
3	9	-4.55	-5.17	0.74	-0.04	-3.81	-5.21
3	10	0.07	0.07	-0.01	-0.02	0.06	0.05

4	5	-3.77	-2.21	-0.05	-0.63	-3.82	-2.84
4	6	-6.69	-6.02	-3.90	-0.78	-10.59	-6.80
4	7	0.07	0.07	-0.01	-0.02	0.06	0.05
4	8	-4.55	-5.17	0.74	-0.04	-3.81	-5.21
4	9	0.07	0.07	-0.01	-0.02	0.06	0.05
4	10	-4.55	-5.17	0.74	-0.04	-3.81	-5.21
5	6	-0.17	-0.01	37.69	36.37	37.52	36.36
5	7	-7.18	-6.47	-0.16	3.04	-7.34	-3.43
5	8	-0.03	-0.02	0.86	1.50	0.83	1.48
5	9	-7.18	-6.47	-0.16	3.04	-7.34	-3.43
5	10	-0.03	-0.02	0.86	1.50	0.83	1.48
6	7	-0.03	-0.02	0.86	1.50	0.83	1.48
6	8	-7.18	-6.47	-0.16	3.04	-7.34	-3.43
6	9	-0.03	-0.02	0.86	1.50	0.83	1.48
6	10	-7.18	-6.47	-0.16	3.04	-7.34	-3.43
7	8	-0.03	-0.04	0.03	0.06	-0.01	0.02
7	9	-4.79	-5.52	0.71	0.17	-4.08	-5.35
7	10	-0.09	-0.10	0.05	0.06	-0.04	-0.04
8	9	-0.09	-0.10	0.05	0.06	-0.04	-0.04
8	10	-4.79	-5.52	0.71	0.17	-4.08	-5.35
9	10	-0.03	-0.04	0.03	0.06	-0.01	0.02

MOLECULE & CALCULATION = NH3_NH3 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	N	-2.98050222	-0.15794358	0.00000000
2	N	2.98050222	0.15794358	0.00000000
3	H	-1.63389015	1.20590889	0.00000000
4	H	1.63389015	-1.20590889	0.00000000
5	H	-4.08412240	0.16220569	1.52992227
6	H	4.08412240	-0.16220569	-1.52992227
7	H	-4.08412240	0.16220569	-1.52992227
8	H	4.08412240	-0.16220569	1.52992227

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.179663	-1.179663	5.969368	0.022706	-1.391605	-1.380252
1	3	-1.179663	0.417409	1.916627	0.679359	0.492402	0.832081
1	4	-1.179663	0.417409	4.731897	0.039080	0.492402	0.511942
1	5	-1.179663	0.381020	1.913409	0.721147	0.449475	0.810049
1	6	-1.179663	0.381020	7.228389	0.001571	0.449475	0.450261
1	7	-1.179663	0.381020	1.913409	0.721147	0.449475	0.810049
1	8	-1.179663	0.381020	7.228389	0.001571	0.449475	0.450261
2	3	-1.179663	0.417409	4.731897	0.039080	0.492402	0.511942
2	4	-1.179663	0.417409	1.916627	0.679359	0.492402	0.832081
2	5	-1.179663	0.381020	7.228389	0.001571	0.449475	0.450261
2	6	-1.179663	0.381020	1.913409	0.721147	0.449475	0.810049
2	7	-1.179663	0.381020	7.228389	0.001571	0.449475	0.450261
2	8	-1.179663	0.381020	1.913409	0.721147	0.449475	0.810049
3	4	0.417409	0.417409	4.061435	0.002236	-0.174230	-0.173112
3	5	0.417409	0.381020	3.071419	0.029224	-0.159041	-0.144429

3	6	0.417409	0.381020	6.075201	-0.001315	-0.159041	-0.159699
3	7	0.417409	0.381020	3.071419	0.029224	-0.159041	-0.144429
3	8	0.417409	0.381020	6.075201	-0.001315	-0.159041	-0.159699
4	5	0.417409	0.381020	6.075201	-0.001315	-0.159041	-0.159699
4	6	0.417409	0.381020	3.071419	0.029224	-0.159041	-0.144429
4	7	0.417409	0.381020	6.075201	-0.001315	-0.159041	-0.159699
4	8	0.417409	0.381020	3.071419	0.029224	-0.159041	-0.144429
5	6	0.381020	0.381020	8.728580	0.001730	-0.145176	-0.144311
5	7	0.381020	0.381020	3.059845	0.032868	-0.145176	-0.128742
5	8	0.381020	0.381020	8.174684	0.003640	-0.145176	-0.143356
6	7	0.381020	0.381020	8.174684	0.003640	-0.145176	-0.143356
6	8	0.381020	0.381020	3.059845	0.032868	-0.145176	-0.128742
7	8	0.381020	0.381020	8.728580	0.001730	-0.145176	-0.144311

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-2.62	-1.19	146.11	146.29	143.49	145.09
1	3	-139.65	-111.21	-136.37	-161.21	-276.02	-272.43
1	4	-4.60	-2.59	-63.06	-65.30	-67.66	-67.89
1	5	-146.20	-118.25	-118.29	-147.41	-264.49	-265.66
1	6	-0.05	-0.07	-41.37	-39.02	-41.42	-39.09
1	7	-146.20	-118.25	-118.29	-147.41	-264.49	-265.66
1	8	-0.05	-0.07	-41.37	-39.02	-41.42	-39.09
2	3	-4.60	-2.59	-63.06	-65.30	-67.66	-67.89
2	4	-139.65	-111.21	-136.37	-161.21	-276.02	-272.43
2	5	-0.05	-0.07	-41.37	-39.02	-41.42	-39.09
2	6	-146.20	-118.25	-118.29	-147.41	-264.49	-265.66
2	7	-0.05	-0.07	-41.37	-39.02	-41.42	-39.09
2	8	-146.20	-118.25	-118.29	-147.41	-264.49	-265.66
3	4	-0.41	-0.17	26.34	26.92	25.92	26.75
3	5	-2.29	-2.99	42.97	32.49	40.68	29.51
3	6	0.06	0.07	17.05	16.43	17.11	16.50
3	7	-2.29	-2.99	42.97	32.49	40.68	29.51
3	8	0.06	0.07	17.05	16.43	17.11	16.50
4	5	0.06	0.07	17.05	16.43	17.11	16.50
4	6	-2.29	-2.99	42.97	32.49	40.68	29.51
4	7	0.06	0.07	17.05	16.43	17.11	16.50
4	8	-2.29	-2.99	42.97	32.49	40.68	29.51
5	6	-0.05	-0.06	11.61	10.44	11.56	10.37
5	7	-2.54	-3.37	40.18	29.77	37.65	26.40
5	8	-0.13	-0.14	12.13	11.14	12.01	11.00
6	7	-0.13	-0.14	12.13	11.14	12.01	11.00
6	8	-2.54	-3.37	40.18	29.77	37.65	26.40
7	8	-0.05	-0.06	11.61	10.44	11.56	10.37

MOLECULE & CALCULATION = FORMALDEHYDE CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	O	0.00000000	0.00000000	1.27736037
2	C	0.00000000	0.00000000	-0.99975961
3	H	0.00000000	1.78182276	-2.11016268

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 4   H      0.00000000   -1.78182276   -2.11016268
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A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.070755	1.139997	2.277120	1.128068	1.220657	1.784691
1	3	-1.070755	-0.034748	3.827559	0.119488	-0.037207	0.022537
1	4	-1.070755	-0.034748	3.827559	0.119488	-0.037207	0.022537
2	3	1.139997	-0.034748	2.099497	0.743210	0.039613	0.411218
2	4	1.139997	-0.034748	2.099497	0.743210	0.039613	0.411218
3	4	-0.034748	-0.034748	3.563646	0.073943	-0.001207	0.035764

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-244.53	-155.43	-557.03	-336.38	-801.55	-491.81
1	3	-10.03	-9.79	-1.58	6.10	-11.61	-3.69
1	4	-10.03	-9.79	-1.58	6.10	-11.61	-3.69
2	3	-153.82	-111.07	23.69	-11.84	-130.12	-122.91
2	4	-153.82	-111.07	23.69	-11.84	-130.12	-122.91
3	4	-5.15	-6.51	0.59	0.21	-4.55	-6.30

MOLECULE & CALCULATION = HF_CLF CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	F	-0.07140217	3.83713853	0.00000000
2	Cl	0.04497195	0.77567374	0.00000000
3	F	0.11652572	-4.66062172	0.00000000
4	H	-1.17063509	-5.77510487	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-0.385869	0.388395	3.063676	0.981424	0.149870	0.640582
1	3	-0.385869	-0.731178	8.499838	0.003512	-0.282139	-0.280383
1	4	-0.385869	0.728515	9.674892	0.003278	0.281111	0.282750
2	3	0.388395	-0.731178	5.436766	0.055107	0.283986	0.311539
2	4	0.388395	0.728515	6.662612	-0.001340	-0.282952	-0.283622
3	4	-0.731178	0.728515	1.702603	0.440068	0.532674	0.752708

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-165.19	-100.51	-43.58	-30.70	-208.77	-131.21
1	3	-0.12	-0.13	19.65	20.83	19.54	20.70
1	4	-0.10	-0.11	-18.12	-18.23	-18.21	-18.34
2	3	-6.50	-3.18	-29.30	-32.78	-35.80	-35.96
2	4	0.09	0.06	25.03	26.65	25.12	26.71
3	4	-93.44	-81.10	-194.23	-196.32	-287.67	-277.42

MOLECULE & CALCULATION = NH3 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	N	0.00000000	0.00000000	0.00000000
2	H	0.00000000	-1.77199619	-0.72111949
3	H	1.53464659	0.88609258	-0.72111949
4	H	-1.53464659	0.88609258	-0.72111949

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-1.152289	0.384166	1.913108	0.720614	0.442670	0.802977
1	3	-1.152289	0.384163	1.913195	0.720613	0.442667	0.802973
1	4	-1.152289	0.384163	1.913195	0.720613	0.442667	0.802973
2	3	0.384166	0.384163	3.069296	0.032879	-0.147582	-0.131143
2	4	0.384166	0.384163	3.069296	0.032879	-0.147582	-0.131143
3	4	0.384163	0.384163	3.069293	0.032881	-0.147581	-0.131141

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-145.97	-118.18	-117.25	-145.20	-263.22	-263.38
1	3	-145.97	-118.18	-117.28	-145.19	-263.25	-263.37
1	4	-145.97	-118.18	-117.28	-145.19	-263.25	-263.37
2	3	-2.52	-3.36	40.58	30.17	38.06	26.81
2	4	-2.52	-3.36	40.58	30.17	38.06	26.81
3	4	-2.52	-3.36	40.58	30.17	38.06	26.81

MOLECULE & CALCULATION = BH3 CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	B	0.00000000	0.00000000	0.00000000
2	H	0.00000000	2.24877409	0.00000000
3	H	1.94755174	-1.12438704	0.00000000
4	H	-1.94755174	-1.12438704	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	2.083826	-0.695010	2.248774	0.472242	1.448280	1.684401
1	3	2.083826	-0.694710	2.248823	0.472166	1.447655	1.683738
1	4	2.083826	-0.694710	2.248823	0.472166	1.447655	1.683738
2	3	-0.695010	-0.694710	3.895019	0.137235	-0.482830	-0.414213
2	4	-0.695010	-0.694710	3.895019	0.137235	-0.482830	-0.414213
3	4	-0.694710	-0.694710	3.895103	0.137112	-0.482622	-0.414066

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-93.17	-65.89	-461.13	-404.14	-554.30	-470.02
1	3	-93.15	-65.88	-460.87	-403.95	-554.02	-469.83
1	4	-93.15	-65.88	-460.87	-403.95	-554.02	-469.83
2	3	-15.89	-11.05	94.01	77.79	78.12	66.73
2	4	-15.89	-11.05	94.01	77.79	78.12	66.73
3	4	-15.87	-11.04	93.95	77.75	78.08	66.71

MOLECULE & CALCULATION = METHANOL CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.03443006	1.26633914	0.00000000
2	O	-0.24080685	-1.41621702	0.00000000
3	H	-1.83059267	2.16664332	0.00000000
4	H	1.07510252	1.86851179	1.68639159
5	H	1.07510252	1.86851179	-1.68639159
6	H	1.40026204	-2.17196558	0.00000000

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.640064	-1.077269	2.696639	0.732267	0.689521	1.055655
1	3	0.640064	-0.021955	2.070956	0.745974	0.014053	0.387040
1	4	0.640064	-0.061898	2.071117	0.745509	0.039619	0.412373
1	5	0.640064	-0.061898	2.071117	0.745509	0.039619	0.412373
1	6	0.640064	0.582282	3.699654	0.012320	-0.372698	-0.366538
2	3	-1.077269	-0.021955	3.919733	0.071772	-0.023651	0.012235
2	4	-1.077269	-0.061898	3.919819	0.077676	-0.066681	-0.027843
2	5	-1.077269	-0.061898	3.919819	0.077676	-0.066681	-0.027843
2	6	-1.077269	0.582282	1.806727	0.565975	0.627274	0.910262
3	4	-0.021955	-0.061898	3.372812	0.059737	-0.001359	0.028510
3	5	-0.021955	-0.061898	3.372812	0.059737	-0.001359	0.028510
3	6	-0.021955	0.582282	5.409432	0.009979	0.012784	0.017774
4	5	-0.061898	-0.061898	3.372783	0.062106	-0.003831	0.027222
4	6	-0.061898	0.582282	4.390342	0.013161	0.036042	0.042623
5	6	-0.061898	0.582282	4.390342	0.013161	0.036042	0.042623

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-159.39	-85.20	-206.52	-160.45	-365.92	-245.65
1	3	-156.53	-113.02	24.05	-4.26	-132.49	-117.27
1	4	-156.88	-112.94	17.23	-12.00	-139.65	-124.94
1	5	-156.88	-112.94	17.23	-12.00	-139.65	-124.94
1	6	-1.26	-1.04	84.20	63.21	82.94	62.17
2	3	-6.63	-5.74	-0.94	3.79	-7.57	-1.96
2	4	-7.13	-6.22	5.58	10.67	-1.55	4.46

2	5	-7.13	-6.22	5.58	10.67	-1.55	4.46
2	6	-118.90	-98.29	-199.31	-217.86	-318.20	-316.15
3	4	-4.92	-5.56	0.64	0.25	-4.29	-5.30
3	5	-4.92	-5.56	0.64	0.25	-4.29	-5.30
3	6	-0.44	-0.58	0.29	-1.48	-0.15	-2.06
4	5	-5.10	-5.78	0.83	0.71	-4.27	-5.06
4	6	-0.86	-0.94	-3.51	-5.15	-4.37	-6.09
5	6	-0.86	-0.94	-3.51	-5.15	-4.37	-6.09

MOLECULE & CALCULATION = ACETYLENE CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	C	0.00000000	0.00000000	1.13629232
2	C	0.00000000	0.00000000	-1.13629232
3	H	0.00000000	0.00000000	3.14526016
4	H	0.00000000	0.00000000	-3.14526016

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	-0.133781	-0.133781	2.272585	1.801607	-0.017897	0.882906
1	3	-0.133781	0.133666	2.008968	0.829512	0.017882	0.432638
1	4	-0.133781	0.133666	4.281552	0.073094	0.017882	0.054429
2	3	-0.133781	0.133666	4.281552	0.073094	0.017882	0.054429
2	4	-0.133781	0.133666	2.008968	0.829512	0.017882	0.432638
3	4	0.133666	0.133666	6.290520	0.017622	-0.017867	-0.009056

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-367.04	-248.73	87.80	4.94	-279.24	-243.79
1	3	-166.45	-129.55	29.47	-5.59	-136.97	-135.14
1	4	-4.56	-5.36	1.34	-2.62	-3.21	-7.98
2	3	-4.56	-5.36	1.34	-2.62	-3.21	-7.98
2	4	-166.45	-129.55	29.47	-5.59	-136.97	-135.14
3	4	-0.74	-0.88	2.57	1.78	1.83	0.90

MOLECULE & CALCULATION = NO_NO CCSD(T)

Atomic coordinates (bohr)

		X	Y	Z
1	N	2.11271381	0.00000000	1.15369040
2	N	-2.11271381	0.00000000	1.15369040
3	O	2.47856478	0.00000000	-1.00947910
4	O	-2.47856478	0.00000000	-1.00947910

A	B	Q^A	Q^B	R^AB	delta^AB	i^AB	e^AB
1	2	0.395440	0.395440	4.225428	0.242191	-0.156373	-0.035277
1	3	0.395440	-0.395128	2.193889	1.550479	0.156249	0.931489
1	4	0.395440	-0.395128	5.075346	0.032811	0.156249	0.172655
2	3	0.395440	-0.395128	5.075346	0.032811	0.156249	0.172655
2	4	0.395440	-0.395128	2.193889	1.550479	0.156249	0.931489
3	4	-0.395128	-0.395128	4.957130	0.104038	-0.156126	-0.104107

A	B	V_xc^AB	V_xc^AB*	V_cl^AB	V_cl^AB*	E_int^AB	E_int^AB*
1	2	-34.67	-17.98	24.99	23.22	-9.67	5.24
1	3	-339.42	-221.74	-11.36	-44.69	-350.77	-266.43
1	4	-2.86	-2.03	-22.19	-19.32	-25.05	-21.35
2	3	-2.86	-2.03	-22.19	-19.32	-25.05	-21.35
2	4	-339.42	-221.74	-11.36	-44.69	-350.77	-266.43
3	4	-10.70	-6.58	20.67	19.76	9.97	13.18

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