Supplements

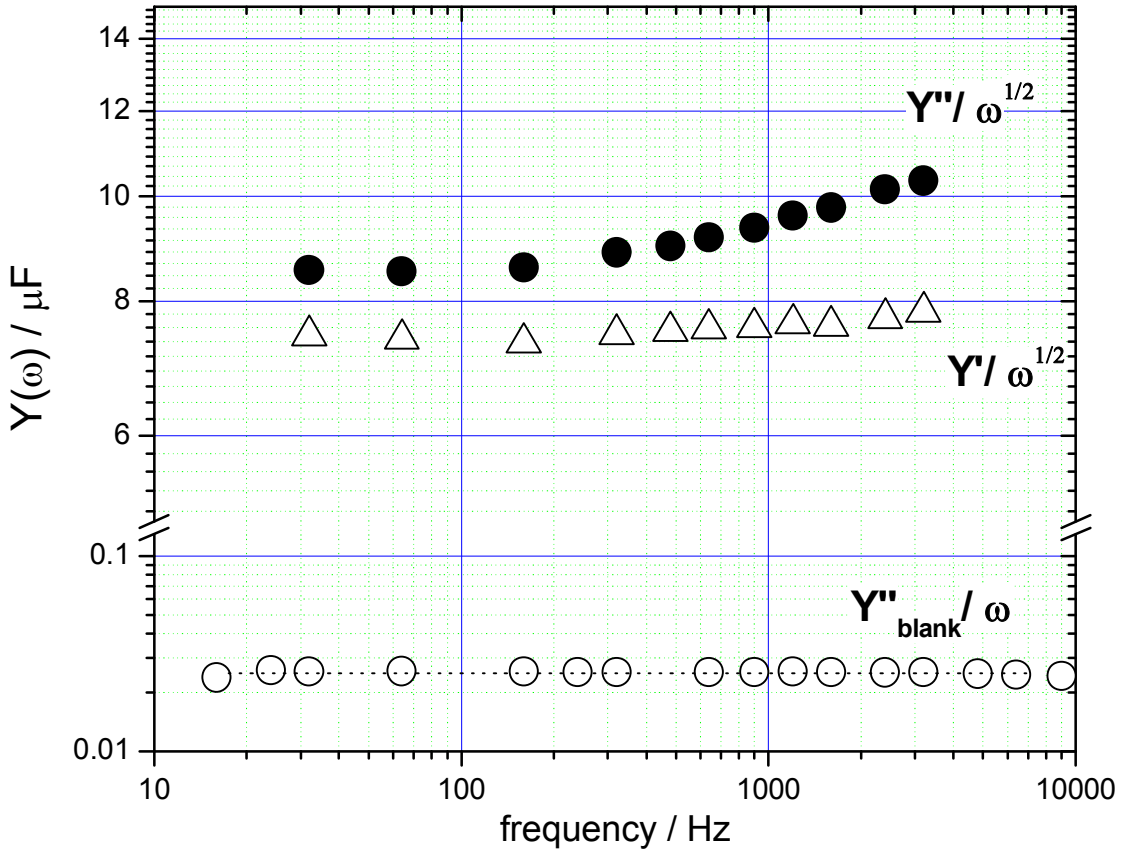
Content:

1. Redox potentials of compounds **1** to **5**

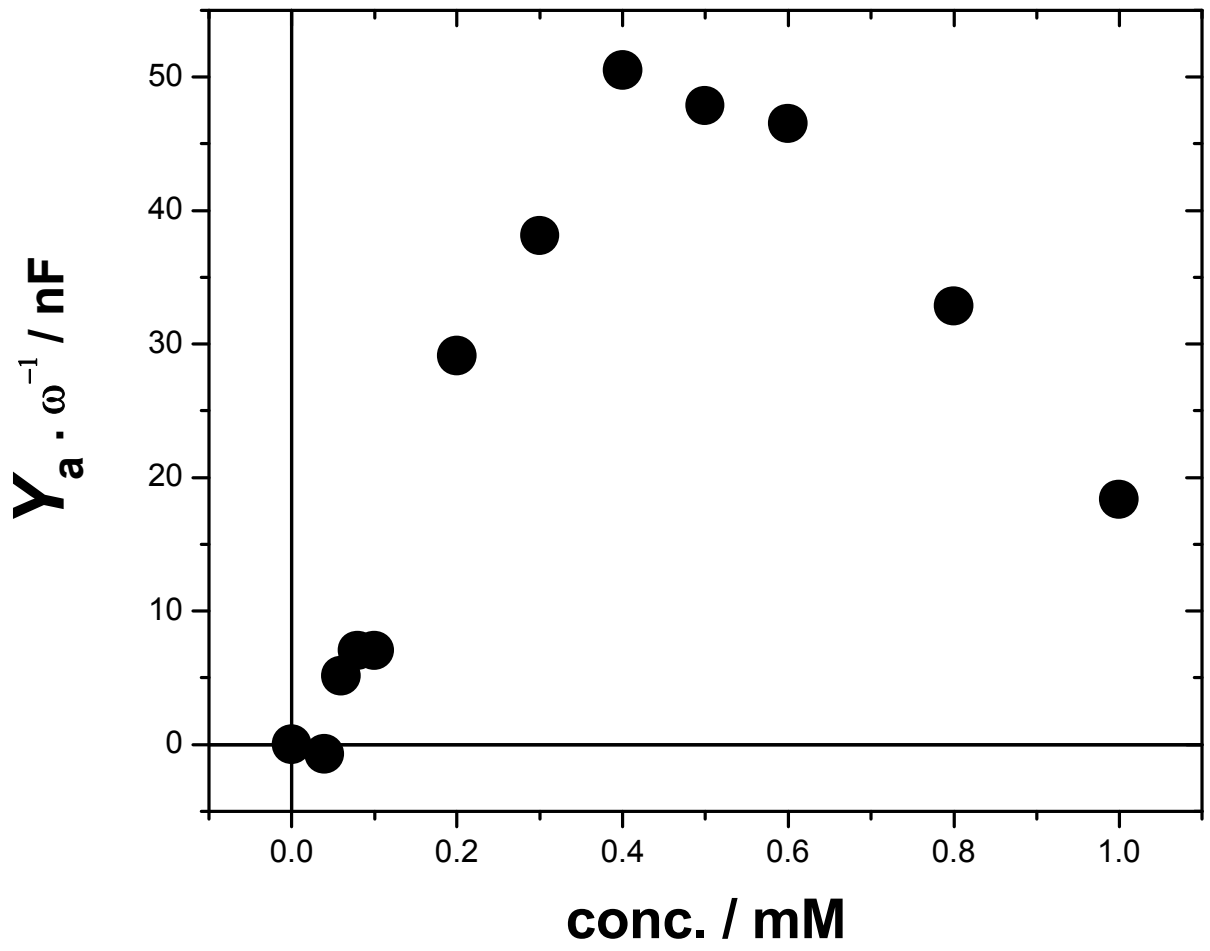
All values are referred to the ferrocene/ferricinium redox couple

Compound	1th redox potl.	2nd redox potl.
1	-1.248	-1.488
2	-1.272	-1.528
3	-1.277	-1.516
4	-1.303	-1.524
5	-1.317	-1.587

2. The frequency dependence of the electrode admittance of the blank and in the presence of 1 mM **1**. Solvent was acetonitrile, the indifferent electrolyte was 0.1 M TBA PF_6 . Circles show the absence of the frequency dispersion of the electrode



3. The concentration dependence of the adsorption contribution to the electrode admittance evaluated as the difference of the imaginary and real admittance components at the frequency of AC signal 160 Hz.



4. SCF calculations, compound **1**

```
+-------------------------------------------------------------------+
|  Jaguar version 3.5, release  42                                  |
|                                                                   |
|  Copyright 1991-1998 Schrodinger, Inc.                            |
|  All Rights Reserved.                                             |
|                                                                   |
|  Use of this program should be acknowledged in publications as:   |
|  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.           |
+-------------------------------------------------------------------+

 start of program pre
 Job name: WF16338
 Executables used: C:\PROGRA~1\WAVEFU~1\TITAN
 Temporary files : C:\DOCUME~1\ADMINI~1\LOCALS~1\Temp\WF16338

 Input file comments:
   Molecule001
   This file created by Spartan

 basis set:              6-31g*
 net molecular charge:    1
 multiplicity:            2

 number of basis functions....          366

Input geometry:
                              angstroms
 atom            x                  y                  z
 H1        4.7248340000      0.1865370000     -1.3549970000
 C1        3.7207930000     -0.2279830000     -1.4028310000
 C2        1.1844900000     -1.2690890000     -1.4270260000
 N2        2.8628370000      0.0719610000     -0.3964410000
 C4        3.3376590000     -1.0510710000     -2.4509030000
 C5        2.0639500000     -1.5922590000     -2.4551130000
 C6        1.5697610000     -0.3786130000     -0.4081170000
 H3        4.0407860000     -1.2929660000     -3.2462420000
 H4        1.7635820000     -2.2751430000     -3.2506980000
 H6        0.2066400000     -1.7444140000     -1.4240300000
 C3        3.3765830000      0.8691880000      0.7469840000
 H7        3.0274740000      1.8970450000      0.5930840000
 H8        4.4710440000      0.8564980000      0.7330540000
 C7        2.8632970000      0.2508320000      2.0370230000
 H11       3.2137580000      0.8493020000      2.8859730000
 H12       3.2372100000     -0.7726250000      2.1576010000
 C9        0.7015310000      0.0175940000      0.7385070000
 C10      -0.7265630000      0.1445230000      0.6993330000
```

```
 C8        1.3546200000      0.2173590000      1.9871420000
 C11      -1.4229540000      0.2251890000      1.9379030000
 H2       -1.2928010000      0.4363990000      4.0957660000
 C12      -0.7469310000      0.3448080000      3.1559640000
 C13       0.6366700000      0.3692670000      3.1772940000
 H16       1.1495560000      0.4912930000      4.1320970000
 C14      -2.9325730000      0.1978140000      1.9420960000
 H9       -3.3064400000      1.2209750000      1.8188990000
 H10      -3.3143240000     -0.1980150000      2.8904050000
 C15      -3.4036060000     -0.6941780000      0.8052120000
 H13      -4.4968850000     -0.6891490000      0.7511960000
 H17      -3.0534000000     -1.7291430000      0.8960700000
 C16      -1.5533260000      0.2721790000     -0.5358660000
 N1       -2.8477760000     -0.1694980000     -0.4686370000
 C18      -3.6694640000     -0.1044330000     -1.5454240000
 H18      -4.6761550000     -0.5017920000     -1.4410580000
 C19      -3.2473450000      0.4661780000     -2.7366170000
 H20      -3.9217770000      0.5222320000     -3.5895320000
 C20      -1.1298130000      0.9149860000     -1.7135720000
 H21      -0.1508090000      1.3828380000     -1.7828510000
 C21      -1.9721570000      0.9977810000     -2.8174080000
 H22      -1.6419760000      1.4875910000     -3.7342370000

 Molecular weight:    286.15 amu

 Stoichiometry:        C20N2H18
 Molecular Point Group: C2
 Point Group used: C1 (symmetry turned off)
 nuclear repulsion energy.......  1732.295717814 hartrees

Non-default options chosen:
  SCF calculation type: RODFT
  RODFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
  Molecular symmetry not used

 end of program pre


 start of program onee
 smallest eigenvalue of S:    2.816E-04
 number of canonical orbitals.....          365
 end of program onee


 start of program hfig
 initial wavefunction generated automatically from atomic wavefunctions
```

Irreducible representation No Symm	Total no orbitals 365	No of occupied orbitals Shell_1 75	Shell_2 1	...
Orbital occupation/shell		1.000	0.500	

end of program hfig

start of program probe
end of program probe

start of program grid

number of gridpoints:

atom	H1	C1	C2	N2	C4	C5	C6	H3
grid # 1	72	85	86	97	89	89	86	73
grid # 2	114	94	96	104	97	96	95	118
grid # 3	216	178	183	215	183	183	189	224
grid # 4	223	314	328	382	331	329	328	232
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	H4	H6	C3	H7	H8	C7	H11	H12
grid # 1	73	71	83	70	68	84	69	70
grid # 2	118	115	91	111	107	92	110	112
grid # 3	222	218	166	220	214	164	215	222
grid # 4	231	222	290	226	219	298	220	226
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C9	C10	C8	C11	H2	C12	C13	H16
grid # 1	93	93	88	88	72	89	89	72
grid # 2	101	101	98	98	116	97	97	116
grid # 3	198	198	195	195	217	186	186	217
grid # 4	346	346	341	341	225	329	329	225
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C14	H9	H10	C15	H13	H17	C16	N1

```
 grid # 1       84     70     69     83     68     70     86     97
 grid # 2       92    112    110     91    107    111     95    104
 grid # 3      164    222    215    166    214    220    189    215
 grid # 4      298    226    220    290    219    226    328    382
 grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
 grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
 grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

 number of gridpoints:
    atom       C18    H18    C19    H20    C20    H21    C21    H22
 grid # 1       85     72     89     73     86     71     89     73
 grid # 2       94    114     97    118     96    115     96    118
 grid # 3      178    216    183    224    183    218    183    222
 grid # 4      314    223    331    232    328    222    329    231
 grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
 grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
 grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

 number of gridpoints:
    atom     total
 grid # 1     3214
 grid # 2     4164
 grid # 3     8016
 grid # 4    11280
 grid # 5   172160
 grid # 6    47680
 grid # 7   209040

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf
number of electrons.....        151
number of alpha electrons....    76
number of beta electrons.....    75
number of orbitals, total....   365
number of core orbitals......    75
number of open shell orbs....     1
number of occupied orbitals..    76
number of virtual orbitals...   289
number of hamiltonians.......     2
number of shells.............     2
SCF type: RODFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
```

	iter	upd	dis	iacut	grid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	5	M	-879.06178045630		3.8E-03	1.2E-01
etot	2	Y	Y	6	M	-881.65545644013	2.6E+00	3.5E-03	7.2E-02
etot	3	Y	Y	6	M	-881.77931148404	1.2E-01	1.8E-03	5.6E-02
etot	4	N	Y	2	U	-882.20221950614	4.2E-01	1.6E-03	1.7E-02
etot	5	Y	Y	6	M	-882.23815585619	3.6E-02	1.2E-03	8.6E-03
etot	6	N	Y	2	U	-882.24314750293	5.0E-03	2.5E-04	6.3E-03
etot	7	Y	Y	6	M	-882.24786725622	4.7E-03	7.5E-05	1.3E-03
etot	8	Y	Y	6	M	-882.24811014201	2.4E-04	2.8E-05	4.9E-04
etot	9	N	N	2	U	-882.24807376991	-3.6E-05	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1732.29571781447	
(E)	Total one-electron terms.....	-4614.25315638775	
(I)	Total two-electron terms.....	1999.70936480337	
(L)	Electronic energy.....	-2614.54379158438	(E+I)
(N)	Total energy.....	-882.24807376991	(A+L)

	Total	Coulomb	Exchange+Corr.
Total two-electron terms	1999.70936480337	2128.55437394246	-128.84500913909
Hamiltonian 1.....	1025.08196151037	1070.94828939001	-45.86632787964
Hamiltonian 2.....	1012.09892961138	1057.60608455245	-45.50715494107

SCFE: SCF energy: RODFT -882.24807376991 hartrees iterations: 9

HOMO energy: -0.23019
LUMO energy: -0.17095

Orbital energies:

-14.53616	-14.53544	-10.37257	-10.37209	-10.36724	-10.36702
-10.35730	-10.35709	-10.32712	-10.32702	-10.32428	-10.32396
-10.32233	-10.32226	-10.31725	-10.31718	-10.31253	-10.31231
-10.31091	-10.31075	-10.29257	-10.29200	-1.12982	-1.12898
-0.98234	-0.95873	-0.95669	-0.92664	-0.91595	-0.90013
-0.88761	-0.85009	-0.84659	-0.79434	-0.78378	-0.77841
-0.76080	-0.74981	-0.74870	-0.69709	-0.67493	-0.66557

```
  -0.64761   -0.63232   -0.62494   -0.61906   -0.61332   -0.59923
  -0.59842   -0.59742   -0.57877   -0.57185   -0.56539   -0.55256
  -0.54725   -0.54623   -0.53900   -0.52442   -0.51153   -0.51079
  -0.50431   -0.49988   -0.49457   -0.49309   -0.48216   -0.47882
  -0.46131   -0.44820   -0.44099   -0.42100   -0.41522   -0.40774
  -0.40022   -0.34502   -0.34357   -0.23019   -0.17095   -0.16241
  -0.13787   -0.10629   -0.08840   -0.03266   -0.02799   -0.01774
  -0.01435   -0.00424

 end of program scf


Total cpu seconds     user:     795.233   user+sys:     795.233
```

5. SCF calculations, compound **2**

```
 +-----------------------------------------------------------------------+
 |  Jaguar version 3.5, release  42                                      |
 |                                                                       |
 |  Copyright 1991-1998 Schrodinger, Inc.                                |
 |  All Rights Reserved.                                                 |
 |                                                                       |
 |  Use of this program should be acknowledged in publications as:       |
 |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.               |
 +-----------------------------------------------------------------------+

 start of program pre
 Job name: WF15023
 Executables used: C:\PROGRA~1\WAVEFU~1\TITAN
 Temporary files : C:\DOCUME~1\pospisil\LOCALS~1\Temp\WF15023

 Input file comments:
   Molecule001
   This file created by Spartan

 basis set:             6-31g*
 net molecular charge:    2
 multiplicity:            1

 number of basis functions....          404

Input geometry:
                                angstroms
 atom            x                  y                  z
 H1        4.6848200000       0.3873470000      -1.3741740000
 C1        3.6883410000      -0.0416040000      -1.4466530000
 C2        1.1725580000      -1.1264510000      -1.5329800000
 N2        2.8391790000       0.1476970000      -0.4073450000
 C4        3.3062640000      -0.7742250000      -2.5598430000
 C5        2.0425050000      -1.3368920000      -2.5974950000
 C6        1.5581420000      -0.3277170000      -0.4394890000
 H3        4.0031140000      -0.9297220000      -3.3816840000
 H4        1.7432510000      -1.9506670000      -3.4475410000
 C3        3.3458170000       0.8467880000       0.7944470000
 H7        2.9613770000       1.8724780000       0.7481240000
 H8        4.4403590000       0.8739460000       0.7634740000
 C7        2.8743890000       0.0888850000       2.0252360000
 H11       3.2385750000       0.6365330000       2.9005790000
 H12       3.2895700000      -0.9254220000       2.0452260000
 C9        0.7015330000      -0.0589700000       0.7549730000
 C10      -0.7241400000       0.0596040000       0.7237680000
 C8        1.3582650000      -0.0011880000       2.0202000000
```

```
 C11      -1.4365730000     -0.0101310000      1.9578720000
 C12      -0.7710760000      0.0084600000      3.2071590000
 C13       0.6377790000     -0.0315760000      3.2383660000
 C14      -2.9513960000     -0.0999320000      1.8944980000
 H9       -3.3672760000      0.9142240000      1.9056660000
 H10      -3.3540980000     -0.6558450000      2.7474740000
 C15      -3.3673590000     -0.8459380000      0.6367420000
 H13      -4.4594280000     -0.8725720000      0.5567800000
 H17      -2.9810120000     -1.8712180000      0.5977900000
 C16      -1.5267450000      0.3399390000     -0.5050450000
 N1       -2.8078370000     -0.1354970000     -0.5345490000
 C18      -3.6098960000      0.0639080000     -1.6087980000
 H18      -4.6085200000     -0.3655120000     -1.5848890000
 C19      -3.1787670000      0.8070600000     -2.6968060000
 H20      -3.8383460000      0.9705490000     -3.5473530000
 C20      -1.0930040000      1.1490130000     -1.5725840000
 C21      -1.9147100000      1.3698010000     -2.6727380000
 H22      -1.5780190000      1.9916150000     -3.5027010000
 C17      -1.5598780000      0.0497780000      4.5015180000
 H14      -1.0327780000      0.6165060000      5.2756770000
 H15      -1.7472750000     -0.9667750000      4.8606790000
 H19      -2.5148140000      0.5702640000      4.3797240000
 C22       1.3681450000     -0.0854320000      4.5661250000
 H5        2.3276640000     -0.6049420000      4.4820250000
 H23       0.8071970000     -0.6594140000      5.3105850000
 H24       1.5391460000      0.9276020000      4.9429740000
 H2        0.2033400000     -1.6186100000     -1.5624630000
 H16      -0.1235440000      1.6412320000     -1.5541510000

 Molecular weight:    314.18 amu

 Stoichiometry:        C22N2H22
 Molecular Point Group: C2
 Point Group used: C1 (symmetry turned off)
 nuclear repulsion energy.......  2027.393825764 hartrees

Non-default options chosen:
  SCF calculation type: DFT
  DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
  Molecular symmetry not used

 end of program pre


 start of program onee
 smallest eigenvalue of S:    2.526E-04
 number of canonical orbitals.....          403
```

```
end of program onee


start of program hfig
initial wavefunction generated automatically from atomic wavefunctions

Irreducible     Total no   No of occupied orbitals
representation  orbitals   Shell_1  Shell_2    ...
No Symm          403         83
------------------------
Orbital occupation/shell    1.000

end of program hfig


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom        H1     C1     C2     N2     C4     C5     C6     H3
grid # 1       72     85     86     96     89     89     86     73
grid # 2      115     94     96    104     97     96     95    118
grid # 3      216    178    183    215    183    183    190    224
grid # 4      223    314    329    382    331    329    330    232
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

number of gridpoints:
   atom        H4     C3     H7     H8     C7    H11    H12     C9
grid # 1       73     83     70     68     84     68     69     93
grid # 2      118     91    111    107     92    107    110    101
grid # 3      222    166    220    214    164    208    218    199
grid # 4      231    288    225    219    298    213    223    346
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

number of gridpoints:
   atom       C10     C8    C11    C12    C13    C14     H9    H10
grid # 1       93     90     90     93     93     84     69     68
grid # 2      101     98     98    101    101     92    110    107
grid # 3      199    196    196    195    195    164    218    208
grid # 4      346    345    345    348    348    298    223    213
```

```
 grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
 grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
 grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

 number of gridpoints:
    atom       C15    H13    H17    C16     N1    C18    H18    C19
 grid # 1       83     68     70     86     96     85     72     89
 grid # 2       91    107    111     95    104     94    115     97
 grid # 3      166    214    220    190    215    178    216    183
 grid # 4      288    219    225    330    382    314    223    331
 grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
 grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
 grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

 number of gridpoints:
    atom       H20    C20    C21    H22    C17    H14    H15    H19
 grid # 1       73     86     89     73     74     69     72     69
 grid # 2      118     96     96    118     82    107    111    107
 grid # 3      224    183    183    222    152    210    216    210
 grid # 4      232    329    329    231    291    215    222    215
 grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
 grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
 grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

 number of gridpoints:
    atom       C22     H5    H23    H24     H2    H16  total
 grid # 1       74     69     69     72     71     71   3644
 grid # 2       82    107    107    111    114    114   4744
 grid # 3      152    210    210    216    217    217   9158
 grid # 4      291    215    215    222    223    223  12744
 grid # 5     4304   4304   4304   4304   4304   4304 197984
 grid # 6     1192   1192   1192   1192   1192   1192  54832
 grid # 7     5226   5226   5226   5226   5226   5226 240396

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf
number of electrons.....        166
number of alpha electrons....    83
number of beta electrons.....    83
number of orbitals, total....   403
number of core orbitals......    83
```

```
 number of open shell orbs....          0
 number of occupied orbitals..         83
 number of virtual orbitals...        320
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
```

	iter	updated	diis	integ.	grid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	5	M	-956.90991687703		5.0E-03	1.2E-01
etot	2	Y	Y	6	M	-959.99909218579	3.1E+00	4.0E-03	6.1E-02
etot	3	Y	Y	6	M	-960.23619181897	2.4E-01	1.8E-03	5.3E-02
etot	4	N	Y	2	U	-960.54855721605	3.1E-01	2.0E-03	2.6E-02
etot	5	Y	Y	6	M	-960.58682580195	3.8E-02	1.9E-03	1.4E-02
etot	6	N	Y	2	U	-960.59849296698	1.2E-02	2.5E-04	4.0E-03
etot	7	Y	Y	6	M	-960.60114922319	2.7E-03	7.5E-05	1.4E-03
etot	8	Y	Y	6	M	-960.60140808225	2.6E-04	3.0E-05	4.1E-04
etot	9	N	N	2	U	-960.60136842640	-4.0E-05	0.0E+00	0.0E+00

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  2027.39382576376
   (E)  Total one-electron terms..... -5284.39289576641
   (I)  Total two-electron terms.....  2296.39770157625
   (J)    Coulomb.....................  2437.26101687410
   (K)    Exchange+Correlation.......  -140.86331529784
   (L)  Electronic energy............. -2987.99519419016  (E+I)
   (N)  Total energy.................  -960.60136842640  (A+L)

 SCFE: SCF energy: DFT    -960.60136842640 hartrees   iterations:   9


 HOMO energy:    -0.46721
 LUMO energy:    -0.32746

  Orbital energies:
  -14.68890  -14.68890  -10.52528  -10.52527  -10.50505  -10.50504
  -10.48037  -10.48037  -10.46697  -10.46697  -10.46669  -10.46669
  -10.46374  -10.46333  -10.45591  -10.45590  -10.44596  -10.44596
  -10.43462  -10.43414  -10.43187  -10.43186  -10.38703  -10.38702
   -1.27496   -1.27401   -1.11710   -1.09592   -1.09540   -1.06469
   -1.05850   -1.03491   -1.01870   -1.00094   -0.98368   -0.93905
   -0.92743   -0.91606   -0.91219   -0.91016   -0.88502   -0.87954
   -0.86245   -0.80702   -0.80130   -0.78900   -0.77863   -0.76580
```

```
 -0.76321   -0.74884   -0.74377   -0.73378   -0.72738   -0.72477
 -0.71323   -0.71129   -0.69283   -0.69012   -0.67531   -0.67002
 -0.65771   -0.64820   -0.64197   -0.64166   -0.63145   -0.63138
 -0.62955   -0.62515   -0.61856   -0.61170   -0.60735   -0.60371
 -0.60183   -0.58559   -0.57449   -0.56331   -0.56041   -0.55672
 -0.55036   -0.54265   -0.52186   -0.46851   -0.46721   -0.32746
 -0.30396   -0.29681   -0.27413   -0.23946   -0.21994   -0.15608
 -0.14859   -0.14257   -0.13264
Total cpu seconds     user:     314.203   user+sys:     314.203
```

6. SCF calculations, compound **4**

```
+-------------------------------------------------------------------+
|  Jaguar version 3.5, release  42                                  |
|                                                                   |
|  Copyright 1991-1998 Schrodinger, Inc.                            |
|  All Rights Reserved.                                             |
|                                                                   |
|  Use of this program should be acknowledged in publications as:   |
|  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.           |
+-------------------------------------------------------------------+

 start of program pre
 Job name: WF12835
 Executables used: C:\PROGRA~1\WAVEFU~1\TITAN
 Temporary files : C:\DOCUME~1\pospisil\LOCALS~1\Temp\WF12835

 Input file comments:
   Molecule001
   This file created by Spartan

 basis set:              6-31g*
 net molecular charge:    2
 multiplicity:            1

 number of basis functions....          442

Input geometry:
                              angstroms
 atom            x                  y                  z
 H1        4.6458310000      0.2076260000     -1.3518190000
 C1        3.6541270000     -0.2324940000     -1.4245390000
 C2        1.1525690000     -1.3931760000     -1.4789870000
 N2        2.8108910000     -0.0690500000     -0.3783190000
 C4        3.2771060000     -0.9511760000     -2.5418620000
 C5        2.0324940000     -1.5536030000     -2.5584010000
 C6        1.5223250000     -0.5404210000     -0.4069670000
 H3        3.9667970000     -1.0842740000     -3.3731160000
 H4        1.7610690000     -2.1803310000     -3.4102490000
 C3        3.3475860000      0.5729740000      0.8465030000
 H7        3.0124640000      1.6166370000      0.8288950000
 H8        4.4424340000      0.5458180000      0.8168940000
 C7        2.8390450000     -0.1999760000      2.0554110000
 H11       3.2495380000      0.2840200000      2.9465330000
 H12       3.1738270000     -1.2432920000      2.0329630000
 C9        0.6800820000     -0.1636790000      0.7733270000
 C10      -0.7060810000      0.1659940000      0.7225620000
 C8        1.3221410000     -0.1621300000      2.0486600000
```

C11	-1.4378470000	0.1724360000	1.9486090000
C12	-0.7987640000	0.1107910000	3.2104070000
C13	0.5943260000	-0.0925840000	3.2610170000
C14	-2.9513290000	0.2099770000	1.8464400000
H9	-3.2834050000	1.2530520000	1.7934110000
H10	-3.4247120000	-0.2684180000	2.7089360000
C15	-3.3721420000	-0.5707870000	0.6091640000
H13	-4.4620500000	-0.5440710000	0.5010300000
H17	-3.0368580000	-1.6144640000	0.6222660000
C16	-1.4615240000	0.5350060000	-0.5174130000
N1	-2.7489400000	0.0635330000	-0.5781370000
C18	-3.5150270000	0.2201060000	-1.6830950000
H18	-4.5094940000	-0.2197680000	-1.6787950000
C19	-3.0587730000	0.9317300000	-2.7751020000
H20	-3.6871150000	1.0593650000	-3.6544580000
C20	-1.0157300000	1.3809880000	-1.5656110000
C21	-1.8160360000	1.5343250000	-2.7062860000
H22	-1.4841430000	2.1556680000	-3.5404830000
C17	-1.5988170000	0.2387830000	4.4930480000
H14	-1.0244170000	0.7448290000	5.2755500000
H15	-1.9002530000	-0.7508720000	4.8495840000
H19	-2.4908680000	0.8590530000	4.3591620000
C22	1.3004140000	-0.2122070000	4.5984650000
H5	2.1996220000	-0.8331140000	4.5327840000
H23	0.6713210000	-0.7133810000	5.3410220000
H24	1.5757620000	0.7797720000	4.9693560000
C23	-0.1182960000	-2.1992420000	-1.5325470000
H16	0.0923450000	-3.2104380000	-1.9014610000
H25	-0.8377940000	-1.7352050000	-2.2134460000
H26	-0.5695990000	-2.3260210000	-0.5452960000
C24	0.2558910000	2.1869880000	-1.5331370000
H6	1.0222100000	1.7187800000	-2.1577720000
H27	0.6353430000	2.3201660000	-0.5169230000
H28	0.0724500000	3.1957610000	-1.9226370000

Molecular weight: 342.21 amu

Stoichiometry: C24N2H26
Molecular Point Group: C2
Point Group used: C1 (symmetry turned off)
nuclear repulsion energy..... 2399.092349529 hartrees

Non-default options chosen:
SCF calculation type: DFT
DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
Molecular symmetry not used

```
end of program pre


start of program onee
smallest eigenvalue of S:    2.550E-04
number of canonical orbitals.....          441
end of program onee


start of program hfig
initial wavefunction generated automatically from atomic wavefunctions

Irreducible     Total no   No of occupied orbitals
representation  orbitals   Shell_1  Shell_2    ...
No Symm          441         91
------------------------
Orbital occupation/shell    1.000

end of program hfig


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom        H1     C1     C2     N2     C4     C5     C6     H3
grid # 1       72     84     89     96     88     88     87     73
grid # 2      114     93    101    104     96     96     96    118
grid # 3      217    178    195    214    182    185    191    222
grid # 4      223    312    343    381    331    330    330    231
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

number of gridpoints:
   atom        H4     C3     H7     H8     C7    H11    H12     C9
grid # 1       72     83     70     68     84     68     69     88
grid # 2      116     91    109    107     92    106    111     98
grid # 3      217    166    216    214    164    209    220    196
grid # 4      224    288    219    219    298    213    224    343
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226
```

number of gridpoints:

atom	C10	C8	C11	C12	C13	C14	H9	H10
grid # 1	88	89	89	92	92	84	69	68
grid # 2	98	98	98	101	101	92	111	106
grid # 3	196	196	196	195	195	164	220	209
grid # 4	343	343	343	347	347	298	224	213
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C15	H13	H17	C16	N1	C18	H18	C19
grid # 1	83	68	70	87	96	84	72	88
grid # 2	91	107	109	96	104	93	114	96
grid # 3	166	214	216	191	214	178	217	182
grid # 4	288	219	219	330	381	312	223	331
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	H20	C20	C21	H22	C17	H14	H15	H19
grid # 1	73	89	88	72	74	69	72	69
grid # 2	118	101	96	116	82	107	111	108
grid # 3	222	195	185	217	152	210	216	211
grid # 4	231	343	330	224	291	215	222	215
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C22	H5	H23	H24	C23	H16	H25	H26
grid # 1	74	69	69	72	72	71	71	69
grid # 2	82	108	107	111	79	109	107	106
grid # 3	152	211	210	216	153	217	216	214
grid # 4	291	215	215	222	294	223	217	215
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C24	H6	H27	H28	total
grid # 1	72	71	69	71	4054
grid # 2	79	107	106	109	5312
grid # 3	153	216	214	217	10332
grid # 4	294	217	215	223	14182
grid # 5	4304	4304	4304	4304	223808

```
 grid # 6     1192   1192   1192   1192  61984
 grid # 7     5226   5226   5226   5226 271752

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf
number of electrons.........        182
number of alpha electrons....         91
number of beta electrons.....         91
number of orbitals, total....        441
number of core orbitals......         91
number of open shell orbs....          0
number of occupied orbitals..         91
number of virtual orbitals...        350
number of hamiltonians.......          1
number of shells.............          1
SCF type: DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)

      i  u  d  i  g
      t  p  i  c  r                              RMS    maximum
      e  d  i  u  i                  energy  density   DIIS
      r  t  s  t  d     total energy change  change    error

etot  1  N  N  5  M -1035.24846968973          5.0E-03  1.2E-01
etot  2  Y  Y  6  M -1038.58371757239  3.3E+00  4.4E-03  7.6E-02
etot  3  Y  Y  6  M -1038.81555929801  2.3E-01  1.9E-03  6.4E-02
etot  4  N  Y  2  U -1039.15303731354  3.4E-01  2.5E-03  2.0E-02
etot  5  Y  Y  6  M -1039.20366631816  5.1E-02  2.4E-03  1.2E-02
etot  6  N  Y  2  U -1039.22167917991  1.8E-02  3.9E-04  6.4E-03
etot  7  Y  Y  6  M -1039.22764870434  6.0E-03  1.1E-04  1.3E-03
etot  8  N  Y  2  U -1039.22789566679  2.5E-04  5.7E-05  6.0E-04
etot  9  Y  N  6  M -1039.22792005479  2.4E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  2399.09234952942
   (E)  Total one-electron terms..... -6128.37546053362
   (I)  Total two-electron terms.....  2690.05519094941
   (J)    Coulomb.....................  2843.28448137341
   (K)    Exchange+Correlation.......  -153.22929042400
   (L)  Electronic energy............. -3438.32026958421  (E+I)
   (N)  Total energy.................. -1039.22792005479  (A+L)
```

```
SCFE: SCF energy: DFT   -1039.22792005479 hartrees   iterations:   9


HOMO energy:    -0.46116
LUMO energy:    -0.32244

 Orbital energies:
 -14.68368  -14.68368  -10.51815  -10.51815  -10.49771  -10.49771
 -10.47713  -10.47713  -10.47187  -10.47187  -10.45914  -10.45913
 -10.45825  -10.45783  -10.45022  -10.45021  -10.43960  -10.43960
 -10.42848  -10.42799  -10.42751  -10.42751  -10.41971  -10.41971
 -10.38302  -10.38302   -1.26831   -1.26728   -1.11248   -1.09580
  -1.09422   -1.06496   -1.05442   -1.03021   -1.01734   -1.00229
  -0.99023   -0.95714   -0.95657   -0.92369   -0.91674   -0.90745
  -0.88859   -0.87860   -0.87641   -0.86218   -0.85865   -0.80141
  -0.79077   -0.78127   -0.76919   -0.76189   -0.76122   -0.74839
  -0.73931   -0.72167   -0.71996   -0.71698   -0.69782   -0.69111
  -0.68469   -0.68254   -0.67252   -0.66977   -0.65687   -0.65509
  -0.65124   -0.64615   -0.63585   -0.63548   -0.63027   -0.62474
  -0.62311   -0.61585   -0.61290   -0.60794   -0.60708   -0.60388
  -0.60033   -0.59952   -0.59721   -0.57660   -0.56973   -0.55821
  -0.55423   -0.54555   -0.53998   -0.52216   -0.51357   -0.46335
  -0.46116   -0.32244   -0.30116   -0.28665   -0.26975   -0.23790
  -0.21942   -0.14535   -0.14374   -0.14310   -0.14068

  Total cpu seconds     user:     409.734   user+sys:     409.734
```

7. SFC calculations compound 5

```
+-------------------------------------------------------------------------+
|  Jaguar version 3.5, release  42                                        |
|                                                                         |
|  Copyright 1991-1998 Schrodinger, Inc.                                  |
|  All Rights Reserved.                                                   |
|                                                                         |
|  Use of this program should be acknowledged in publications as:         |
|  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.                 |
+-------------------------------------------------------------------------+

 start of program pre
 Job name: WF12835
 Executables used: C:\PROGRA~1\WAVEFU~1\TITAN
 Temporary files : C:\DOCUME~1\pospisil\LOCALS~1\Temp\WF12835

 Input file comments:
   Molecule001
   This file created by Spartan

 basis set:              6-31g*
 net molecular charge:     2
 multiplicity:             1

 number of basis functions....          442

Input geometry:
                                angstroms
 atom            x                  y                  z
 H1        4.6458310000       0.2076260000      -1.3518190000
 C1        3.6541270000      -0.2324940000      -1.4245390000
 C2        1.1525690000      -1.3931760000      -1.4789870000
 N2        2.8108910000      -0.0690500000      -0.3783190000
 C4        3.2771060000      -0.9511760000      -2.5418620000
 C5        2.0324940000      -1.5536030000      -2.5584010000
 C6        1.5223250000      -0.5404210000      -0.4069670000
 H3        3.9667970000      -1.0842740000      -3.3731160000
 H4        1.7610690000      -2.1803310000      -3.4102490000
 C3        3.3475860000       0.5729740000       0.8465030000
 H7        3.0124640000       1.6166370000       0.8288950000
 H8        4.4424340000       0.5458180000       0.8168940000
 C7        2.8390450000      -0.1999760000       2.0554110000
 H11       3.2495380000       0.2840200000       2.9465330000
 H12       3.1738270000      -1.2432920000       2.0329630000
 C9        0.6800820000      -0.1636790000       0.7733270000
 C10      -0.7060810000       0.1659940000       0.7225620000
```

C8	1.3221410000	-0.1621300000	2.0486600000
C11	-1.4378470000	0.1724360000	1.9486090000
C12	-0.7987640000	0.1107910000	3.2104070000
C13	0.5943260000	-0.0925840000	3.2610170000
C14	-2.9513290000	0.2099770000	1.8464400000
H9	-3.2834050000	1.2530520000	1.7934110000
H10	-3.4247120000	-0.2684180000	2.7089360000
C15	-3.3721420000	-0.5707870000	0.6091640000
H13	-4.4620500000	-0.5440710000	0.5010300000
H17	-3.0368580000	-1.6144640000	0.6222660000
C16	-1.4615240000	0.5350060000	-0.5174130000
N1	-2.7489400000	0.0635330000	-0.5781370000
C18	-3.5150270000	0.2201060000	-1.6830950000
H18	-4.5094940000	-0.2197680000	-1.6787950000
C19	-3.0587730000	0.9317300000	-2.7751020000
H20	-3.6871150000	1.0593650000	-3.6544580000
C20	-1.0157300000	1.3809880000	-1.5656110000
C21	-1.8160360000	1.5343250000	-2.7062860000
H22	-1.4841430000	2.1556680000	-3.5404830000
C17	-1.5988170000	0.2387830000	4.4930480000
H14	-1.0244170000	0.7448290000	5.2755500000
H15	-1.9002530000	-0.7508720000	4.8495840000
H19	-2.4908680000	0.8590530000	4.3591620000
C22	1.3004140000	-0.2122070000	4.5984650000
H5	2.1996220000	-0.8331140000	4.5327840000
H23	0.6713210000	-0.7133810000	5.3410220000
H24	1.5757620000	0.7797720000	4.9693560000
C23	-0.1182960000	-2.1992420000	-1.5325470000
H16	0.0923450000	-3.2104380000	-1.9014610000
H25	-0.8377940000	-1.7352050000	-2.2134460000
H26	-0.5695990000	-2.3260210000	-0.5452960000
C24	0.2558910000	2.1869880000	-1.5331370000
H6	1.0222100000	1.7187800000	-2.1577720000
H27	0.6353430000	2.3201660000	-0.5169230000
H28	0.0724500000	3.1957610000	-1.9226370000

Molecular weight: 342.21 amu

Stoichiometry: C24N2H26
Molecular Point Group: C2
Point Group used: C1 (symmetry turned off)
nuclear repulsion energy..... 2399.092349529 hartrees

Non-default options chosen:
SCF calculation type: DFT
DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)
Molecular symmetry not used

```
end of program pre


start of program onee
smallest eigenvalue of S:    2.550E-04
number of canonical orbitals.....          441
end of program onee


start of program hfig
initial wavefunction generated automatically from atomic wavefunctions

Irreducible     Total no   No of occupied orbitals
representation  orbitals   Shell_1  Shell_2    ...
No Symm          441         91
------------------------
Orbital occupation/shell    1.000

end of program hfig


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom        H1     C1     C2     N2     C4     C5     C6     H3
grid # 1       72     84     89     96     88     88     87     73
grid # 2      114     93    101    104     96     96     96    118
grid # 3      217    178    195    214    182    185    191    222
grid # 4      223    312    343    381    331    330    330    231
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226

number of gridpoints:
   atom        H4     C3     H7     H8     C7    H11    H12     C9
grid # 1       72     83     70     68     84     68     69     88
grid # 2      116     91    109    107     92    106    111     98
grid # 3      217    166    216    214    164    209    220    196
grid # 4      224    288    219    219    298    213    224    343
grid # 5     4304   4304   4304   4304   4304   4304   4304   4304
grid # 6     1192   1192   1192   1192   1192   1192   1192   1192
grid # 7     5226   5226   5226   5226   5226   5226   5226   5226
```

number of gridpoints:

atom	C10	C8	C11	C12	C13	C14	H9	H10
grid # 1	88	89	89	92	92	84	69	68
grid # 2	98	98	98	101	101	92	111	106
grid # 3	196	196	196	195	195	164	220	209
grid # 4	343	343	343	347	347	298	224	213
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C15	H13	H17	C16	N1	C18	H18	C19
grid # 1	83	68	70	87	96	84	72	88
grid # 2	91	107	109	96	104	93	114	96
grid # 3	166	214	216	191	214	178	217	182
grid # 4	288	219	219	330	381	312	223	331
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	H20	C20	C21	H22	C17	H14	H15	H19
grid # 1	73	89	88	72	74	69	72	69
grid # 2	118	101	96	116	82	107	111	108
grid # 3	222	195	185	217	152	210	216	211
grid # 4	231	343	330	224	291	215	222	215
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C22	H5	H23	H24	C23	H16	H25	H26
grid # 1	74	69	69	72	72	71	71	69
grid # 2	82	108	107	111	79	109	107	106
grid # 3	152	211	210	216	153	217	216	214
grid # 4	291	215	215	222	294	223	217	215
grid # 5	4304	4304	4304	4304	4304	4304	4304	4304
grid # 6	1192	1192	1192	1192	1192	1192	1192	1192
grid # 7	5226	5226	5226	5226	5226	5226	5226	5226

number of gridpoints:

atom	C24	H6	H27	H28	total
grid # 1	72	71	69	71	4054
grid # 2	79	107	106	109	5312
grid # 3	153	216	214	217	10332
grid # 4	294	217	215	223	14182

```
  grid # 5     4304   4304   4304   4304 223808
  grid # 6     1192   1192   1192   1192  61984
  grid # 7     5226   5226   5226   5226 271752

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
 number of electrons.........        182
 number of alpha electrons....         91
 number of beta electrons.....         91
 number of orbitals, total....        441
 number of core orbitals......         91
 number of open shell orbs....          0
 number of occupied orbitals..         91
 number of virtual orbitals...        350
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)

       i  u  d  i  g                                        RMS    maximum
       t  p  i  c  r                                    density   DIIS
       e  d  i  u  i                    energy  energy  change    error
       r  t  s  t  d     total energy    change  change  error

etot   1  N  N  5  M -1035.24846968973           5.0E-03  1.2E-01
etot   2  Y  Y  6  M -1038.58371757239  3.3E+00  4.4E-03  7.6E-02
etot   3  Y  Y  6  M -1038.81555929801  2.3E-01  1.9E-03  6.4E-02
etot   4  N  Y  2  U -1039.15303731354  3.4E-01  2.5E-03  2.0E-02
etot   5  Y  Y  6  M -1039.20366631816  5.1E-02  2.4E-03  1.2E-02
etot   6  N  Y  2  U -1039.22167917991  1.8E-02  3.9E-04  6.4E-03
etot   7  Y  Y  6  M -1039.22764870434  6.0E-03  1.1E-04  1.3E-03
etot   8  N  Y  2  U -1039.22789566679  2.5E-04  5.7E-05  6.0E-04
etot   9  Y  N  6  M -1039.22792005479  2.4E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  2399.09234952942
   (E)  Total one-electron terms..... -6128.37546053362
   (I)  Total two-electron terms.....  2690.05519094941
   (J)    Coulomb.....................  2843.28448137341
   (K)    Exchange+Correlation.......  -153.22929042400
   (L)  Electronic energy............. -3438.32026958421  (E+I)
```

```
  (N)  Total energy.................. -1039.22792005479  (A+L)

SCFE: SCF energy: DFT   -1039.22792005479 hartrees   iterations:   9


HOMO energy:    -0.46116
LUMO energy:    -0.32244

 Orbital energies:
 -14.68368  -14.68368  -10.51815  -10.51815  -10.49771  -10.49771
 -10.47713  -10.47713  -10.47187  -10.47187  -10.45914  -10.45913
 -10.45825  -10.45783  -10.45022  -10.45021  -10.43960  -10.43960
 -10.42848  -10.42799  -10.42751  -10.42751  -10.41971  -10.41971
 -10.38302  -10.38302   -1.26831   -1.26728   -1.11248   -1.09580
  -1.09422   -1.06496   -1.05442   -1.03021   -1.01734   -1.00229
  -0.99023   -0.95714   -0.95657   -0.92369   -0.91674   -0.90745
  -0.88859   -0.87860   -0.87641   -0.86218   -0.85865   -0.80141
  -0.79077   -0.78127   -0.76919   -0.76189   -0.76122   -0.74839
  -0.73931   -0.72167   -0.71996   -0.71698   -0.69782   -0.69111
  -0.68469   -0.68254   -0.67252   -0.66977   -0.65687   -0.65509
  -0.65124   -0.64615   -0.63585   -0.63548   -0.63027   -0.62474
  -0.62311   -0.61585   -0.61290   -0.60794   -0.60708   -0.60388
  -0.60033   -0.59952   -0.59721   -0.57660   -0.56973   -0.55821
  -0.55423   -0.54555   -0.53998   -0.52216   -0.51357   -0.46335
  -0.46116   -0.32244   -0.30116   -0.28665   -0.26975   -0.23790
  -0.21942   -0.14535   -0.14374   -0.14310   -0.14068

  Total cpu seconds     user:     409.734   user+sys:     409.734
```