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

On the performance of second-order approximate coupled-cluster singles and doubles methods for non-valence anions

Supplementary Information

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1 Cartesian geometries in Angstrom

1.1 Valence anions

```
$comment
Tetrafluorobenzoquinone
Nuclear Repulsion Energy = 704.26826452 hartrees
$end

$molecule
0 1
  F   2.3756498080  -1.3751980891   0.0000000000
  F   2.3756498080   1.3751980891   0.0000000000
  F  -2.3756498080   1.3751980891   0.0000000000
  F  -2.3756498080  -1.3751980891  -0.0000000000
  C   1.2596187001  -0.6724175000  -0.0000000000
  C   1.2596187001   0.6724175000   0.0000000000
  C  -1.2596187001   0.6724175000  -0.0000000000
  C  -1.2596187001  -0.6724175000  -0.0000000000
  C   0.0000000000   1.4497959443   0.0000000000
  C  -0.0000000000  -1.4497959443  -0.0000000000
  O   0.0000000000   2.6684619443   0.0000000000
  O  -0.0000000000  -2.6684619443  -0.0000000000
$end
```

```
$comment
Benzoquinone
Nuclear Repulsion Energy = 322.80928840 hartrees
$end

$molecule
0 1
  H   1.2522467586   2.1752956190   0.0000000000
  H  -1.2522467586   2.1752956190  -0.0000000000
  H  -1.2522467586  -2.1752956190   0.0000000000
  H   1.2522467586  -2.1752956190  -0.0000000000
  C  -0.6722520106   1.2624676881  -0.0000000000
  C   0.6722520106   1.2624676881   0.0000000000
  C  -0.6722520106  -1.2624676881   0.0000000000
  C   0.6722520106  -1.2624676881  -0.0000000000
  C  -1.4384853819  -0.0000000012   0.0000000000
  C   1.4384853819   0.0000000012   0.0000000000
  O  -2.6663113819   0.0000000032  -0.0000000000
  O   2.6663113819   0.0000000000   0.0000000000
$end


$comment
p-Nitrobenzonitrile
Nuclear Repulsion Energy = 529.48488835 hartrees
$end

$molecule
0 1
  N   0.0000000000   0.0000000000   2.4489844499
  O   1.0918208133  -0.0000000000   3.0112781895
  O  -1.0918208133   0.0000000000   3.0112781895
  C   0.0000000000   0.0000000000   0.9776524499
  C   1.2185899629  -0.0000000000   0.3108953662
  H   2.1368448435  -0.0000000000   0.8768880604
  C   1.2154656969  -0.0000000000  -1.0772231179
  H   2.1459021497  -0.0000000000  -1.6265378249
  C  -1.2185899629   0.0000000000   0.3108953662
  H  -2.1368448435   0.0000000000   0.8768880604
  C  -1.2154656969   0.0000000000  -1.0772231179
  H  -2.1459021497   0.0000000000  -1.6265378249
  C   0.0000000000   0.0000000000  -1.7731871363
  C   0.0000000000   0.0000000000  -3.2030041363
  N   0.0000000000   0.0000000000  -4.3766971363
$end
```

```
$comment
1,4-Naphthoquinone
Nuclear Repulsion Energy = 623.53248846 hartrees
$end

$molecule
0 1
  C  -0.7013334144  -0.0000000000  -0.2560870783
  C  -1.3980277754  -0.0000000000  -1.4658679583
  H  -2.4788243060  -0.0000000000  -1.4384597806
  C  -0.6990446880  -0.0000000000  -2.6670143525
  H  -1.2380846413  -0.0000000000  -3.6043603426
  C   0.6990446880   0.0000000000  -2.6670143525
  H   1.2380846413   0.0000000000  -3.6043603426
  C   1.3980277754   0.0000000000  -1.4658679583
  H   2.4788243060   0.0000000000  -1.4384597806
  C   0.7013334144   0.0000000000  -0.2560870783
  C  -1.4570676272   0.0000000000   1.0210353373
  O  -2.6837070586   0.0000000000   1.0540261569
  C  -0.6725512597   0.0000000000   2.2714989216
  H  -1.2456793580   0.0000000000   3.1892137877
  C   0.6725512597  -0.0000000000   2.2714989216
  H   1.2456793580  -0.0000000000   3.1892137877
  C   1.4570676272  -0.0000000000   1.0210353373
  O   2.6837070586  -0.0000000000   1.0540261569
$end


$comment
Maleic Anhydride
Nuclear Repulsion Energy = 275.04298010 hartrees
$end

$molecule
0 1
  O   0.0000000000   0.0000000000   0.9718680070
  C  -1.1268660872  -0.0000000000   0.1576890229
  C   1.1268660872   0.0000000000   0.1576890229
  O  -2.2395980384  -0.0000000000   0.5973627979
  O   2.2395980384   0.0000000000   0.5973627979
  C  -0.6678593576  -0.0000000000  -1.2547634396
  C   0.6678593576   0.0000000000  -1.2547634396
  H  -1.3552061648  -0.0000000000  -2.0839290906
  H   1.3552061648   0.0000000000  -2.0839290906
$end
```

```
$comment
Phenazine
Nuclear Repulsion Energy = 780.72543176 hartrees
$end

$molecule
0 1
  N   0.0000000000  -1.4328650242   0.0000000000
  C  -1.1407560176  -0.7205037326  -0.0000000000
  C   1.1407560176  -0.7205037326   0.0000000000
  C  -2.3804840748  -1.4116393984  -0.0000000000
  H  -2.3546309664  -2.4927823331  -0.0000000000
  C  -3.5592048726  -0.7099210621  -0.0000000000
  H  -4.5011369865  -1.2414092426  -0.0000000000
  C   2.3804840748  -1.4116393984   0.0000000000
  H   2.3546309664  -2.4927823331   0.0000000000
  C   3.5592048726  -0.7099210621   0.0000000000
  H   4.5011369865  -1.2414092426   0.0000000000
  C   3.5592048726   0.7099210621  -0.0000000000
  H   4.5011369865   1.2414092426  -0.0000000000
  C   2.3804840748   1.4116393984  -0.0000000000
  H   2.3546309664   2.4927823331  -0.0000000000
  C   1.1407560176   0.7205037326  -0.0000000000
  N  -0.0000000029   1.4328650242  -0.0000000000
  C  -1.1407560176   0.7205037326  -0.0000000000
  C  -2.3804840748   1.4116393984  -0.0000000000
  H  -2.3546309664   2.4927823331  -0.0000000000
  C  -3.5592048726   0.7099210621  -0.0000000000
  H  -4.5011369865   1.2414092426  -0.0000000000
$end


$comment
Fumaronitrile
Nuclear Repulsion Energy = 162.78773538 hartrees
$end

$molecule
0 1
  C   0.4866183375   0.4604063019  -0.0000000000
  C  -0.4866183375  -0.4604063019  -0.0000000000
  H   0.2539941120   1.5174807823   0.0000000000
  H  -0.2539941120  -1.5174807823  -0.0000000000
  C   1.8636261111   0.1123116934  -0.0000000000
  C  -1.8636261111  -0.1123116934   0.0000000000
  N   2.9877495396  -0.1427508309  -0.0000000000
  N  -2.9877495396   0.1427508309   0.0000000000
$end
```

```
$comment
Azulene
Nuclear Repulsion Energy = 454.46094658 hartrees
$end
$molecule
0 1
  C  -0.7487798402  -0.0000000000   0.5511274366
  C  -1.5947707452  -0.0000000000  -0.5483651878
  H  -2.6563583743  -0.0000000000  -0.3181972367
  C  -1.2628648085  -0.0000000000  -1.9039171278
  H  -2.1004885786  -0.0000000000  -2.5907702075
  C   0.0000000000   0.0000000000  -2.4969737813
  H   0.0000000000   0.0000000000  -3.5812257813
  C   1.2628648085   0.0000000000  -1.9039171278
  H   2.1004885786   0.0000000000  -2.5907702075
  C   1.5947707452   0.0000000000  -0.5483651878
  H   2.6563583743   0.0000000000  -0.3181972367
  C   0.7487798402   0.0000000000   0.5511274366
  C   1.1497185402   0.0000000000   1.8950553835
  H   2.1735164154   0.0000000000   2.2369636373
  C  -1.1497185402  -0.0000000000   1.8950553835
  H  -2.1735164154  -0.0000000000   2.2369636373
  C   0.0000000000   0.0000000000   2.6999190230
  H   0.0000000000   0.0000000000   3.7807540230
$end

$comment
Isophthalonitrile
Nuclear Repulsion Energy = 408.25362299 hartrees
$end
$molecule
0 1
  C   0.0000000000   0.0000000000  -0.7611454554
  C   0.0000000000   0.0000000000   2.0357668855
  H   0.0000000000   0.0000000000  -1.8416384554
  H   0.0000000000   0.0000000000   3.1163608855
  C   1.2036616314   0.0000000000  -0.0532329145
  C  -1.2036616314  -0.0000000000  -0.0532329145
  C   1.2077592756   0.0000000000   1.3459900855
  C  -1.2077592756  -0.0000000000   1.3459900855
  H   2.1491100458   0.0000000000   1.8765262681
  H  -2.1491100458  -0.0000000000   1.8765262681
  C  -2.4431040460  -0.0000000000  -0.7688835877
  C   2.4431040460   0.0000000000  -0.7688835877
  N  -3.4594892826  -0.0000000000  -1.3544276927
  N   3.4594892826   0.0000000000  -1.3544276927
$end
```

```
$comment
Phthalimide
Nuclear Repulsion Energy = 555.99908405 hartrees
$end

$molecule
0 1
  N   0.0000000000   0.0000000000   2.0040908542
  H   0.0000000000   0.0000000000   3.0119678542
  C   1.1682524528   0.0000000000   1.2386306388
  O   2.3011200960   0.0000000000   1.6670025478
  C  -1.1682524528  -0.0000000000   1.2386306388
  O  -2.3011200960  -0.0000000000   1.6670025478
  C   0.6962780385   0.0000000000  -0.1738809943
  C   1.4225683398   0.0000000000  -1.3533552596
  H   2.5035811189   0.0000000000  -1.3406024073
  C  -0.6962780385  -0.0000000000  -0.1738809943
  C  -1.4225683398  -0.0000000000  -1.3533552596
  H  -2.5035811189  -0.0000000000  -1.3406024073
  C   0.6998855532  -0.0000000000  -2.5485997635
  H   1.2273446728  -0.0000000000  -3.4924903968
  C  -0.6998855532   0.0000000000  -2.5485997635
  H  -1.2273446728   0.0000000000  -3.4924903968
$end


$comment
Phthalic Anhydride
Nuclear Repulsion Energy = 557.95918775 hartrees
$end

$molecule
0 1
  O   0.0000000000   0.0000000000   2.0399909960
  C   1.1433631827   0.0000000000   1.2374942246
  O   2.2469461705   0.0000000000   1.7004541646
  C  -1.1433631827  -0.0000000000   1.2374942246
  O  -2.2469461705  -0.0000000000   1.7004541646
  C   0.6932996629   0.0000000000  -0.1712514501
  C  -0.6932996629  -0.0000000000  -0.1712514501
  C   1.4256099915  -0.0000000000  -1.3488266847
  H   2.5063094367  -0.0000000000  -1.3365653369
  C  -1.4256099915   0.0000000000  -1.3488266847
  H  -2.5063094367   0.0000000000  -1.3365653369
  C   0.7008829906  -0.0000000000  -2.5409864852
  H   1.2267774977  -0.0000000000  -3.4856261389
  C  -0.7008829906   0.0000000000  -2.5409864852
  H  -1.2267774977   0.0000000000  -3.4856261389
$end
```

```
$comment
Acridine
Nuclear Repulsion Energy = 774.34300516 hartrees
$end

$molecule
0 1
  N   0.0000000000   0.0000000000   1.3879036199
  C  -1.1517901135   0.0000000000   0.6929070436
  C   1.1517901135  -0.0000000000   0.6929070436
  C  -2.3720383668   0.0000000000   1.4210815022
  H  -2.3090032869   0.0000000000   2.5007860171
  C  -3.5773593832   0.0000000000   0.7659198613
  H  -4.4988755255   0.0000000000   1.3320183983
  C  -3.6272428692   0.0000000000  -0.6520339617
  H  -4.5863609808   0.0000000000  -1.1520693349
  C  -2.4723143512   0.0000000000  -1.3920873795
  H  -2.5074729570   0.0000000000  -2.4745745637
  C  -1.2067024347   0.0000000000  -0.7460405285
  C   0.0000000000   0.0000000000  -1.4456554735
  H   0.0000000000   0.0000000000  -2.5306814735
  C   1.2067024347  -0.0000000000  -0.7460405285
  C   2.4723143512  -0.0000000000  -1.3920873795
  H   2.5074729570  -0.0000000000  -2.4745745637
  C   3.6272428692  -0.0000000000  -0.6520339617
  H   4.5863609808  -0.0000000000  -1.1520693349
  C   3.5773593832  -0.0000000000   0.7659198613
  H   4.4988755255  -0.0000000000   1.3320183983
  C   2.3720383668  -0.0000000000   1.4210815022
  H   2.3090032869  -0.0000000000   2.5007860171
$end
```

1.2 Dipole-bound radical anions

```
$comment
Uracil
Nuclear Repulsion Energy = 357.68565001 hartrees
$end

$molecule
0 1
  N   0.0332959514  -0.9844726412  -0.0000000000
  H   0.0408384309  -1.9925844260  -0.0000000000
  C  -1.2142801248  -0.3986739772  -0.0000000000
  O  -2.2485813820  -1.0256366008  -0.0000000000
  N  -1.1732974436   0.9814346613  -0.0000000000
  H  -2.0672060280   1.4383995864  -0.0000000000
  C  -0.0016908524   1.7029578150   0.0000000000
  H  -0.1210696066   2.7762189796   0.0000000000
  C   1.2008283331   1.1078262041   0.0000000000
  H   2.1183176446   1.6709330293   0.0000000000
  C   1.2806948986  -0.3510959060   0.0000000000
  O   2.3005584418  -1.0040866649   0.0000000000
$end
```

```
$comment
Nitrobenzene
Nuclear Repulsion Energy = 412.90658632 hartrees
$end

$molecule
0 1
  N   1.7144026049   0.0000137940  -0.0000000000
  O   2.2802741567   1.0903202788  -0.0000000000
  O   2.2803868733  -1.0902736184   0.0000000000
  C   0.2431236050   0.0000260044   0.0000000000
  C  -0.4233660621  -1.2178234556   0.0000000000
  H   0.1431406155  -2.1356344152   0.0000000000
  C  -0.4234525589   1.2178406635  -0.0000000000
  H   0.1429923777   2.1356909042  -0.0000000000
  C  -1.8150472244   1.2073775391  -0.0000000000
  H  -2.3542471026   2.1440765841  -0.0000000000
  C  -1.8149612385  -1.2074285069   0.0000000000
  H  -2.3541011991  -2.1441643479   0.0000000000
  C  -2.5115278990  -0.0000495781  -0.0000000000
  H  -3.5925028981  -0.0000945653  -0.0000000000
$end
```

```
$comment
Benzaldehyde
Nuclear Repulsion Energy = 321.40219102 hartrees
$end

$molecule
0 1
  C   0.5301108806   0.2094451563   0.0000000000
  C  -0.3561025276   1.2878987258   0.0000000000
  H   0.0337637693   2.2985700364   0.0000000000
  C  -1.7292609981   1.0596326904   0.0000000000
  H  -2.4189625404   1.8921549526   0.0000000000
  C  -2.2126128958  -0.2474932818  -0.0000000000
  H  -3.2790500662  -0.4271549301  -0.0000000000
  C  -1.3251205424  -1.3262390907  -0.0000000000
  H  -1.7074112086  -2.3376495336  -0.0000000000
  C   0.0454387787  -1.1012839797  -0.0000000000
  H   0.7548324413  -1.9175156707  -0.0000000000
  C   1.9851692041   0.4694899904   0.0000000000
  H   2.2615603161   1.5403494543   0.0000000000
  O   2.8411919865  -0.3946819466  -0.0000000000
$end


$comment
Benzonitrile
Nuclear Repulsion Energy = 300.09121671 hartrees
$end

$molecule
0 1
  C   0.0000000000  0.0000000000   2.1746561879
  C   1.2072838898  0.0000000000   1.4803615442
  C   1.2122184965  0.0000000000   0.0906046613
  C   0.0000000000  0.0000000000  -0.6023344411
  C  -1.2122184965  0.0000000000   0.0906046613
  C  -1.2072838898  0.0000000000   1.4803615442
  H   0.0000000000  0.0000000000   3.2560219551
  H   2.1441224787  0.0000000000   2.0195328576
  H   2.1428929996  0.0000000000  -0.4589656243
  H  -2.1428929996  0.0000000000  -0.4589656243
  H  -2.1441224787  0.0000000000   2.0195328576
  C   0.0000000000  0.0000000000  -2.0438027391
  N   0.0000000000  0.0000000000  -3.1999807046
$end
```

```
$comment
Phenyl isocyanide
Nuclear Repulsion Energy = 303.79558941 hartrees
$end

$molecule
0 1
  H  -2.1449100000   0.0000000000  -1.9838914815
  C  -1.2075000000   0.0000000000  -1.4459614815
  C   0.0000000000   0.0000000000  -2.1422714815
  H   0.0000000000   0.0000000000  -3.2230614815
  C   1.2075000000  -0.0000000000  -1.4459614815
  H   2.1449100000  -0.0000000000  -1.9838914815
  C   1.2153200000  -0.0000000000  -0.0552214815
  H   2.1396200000  -0.0000000000   0.5041385185
  C  -0.0000000000   0.0000000000   0.6290385185
  C  -1.2153200000   0.0000000000  -0.0552214815
  H  -2.1396200000   0.0000000000   0.5041385185
  N  -0.0000000000   0.0000000000   2.0132985185
  C   0.0000000000   0.0000000000   3.1971785185
$end


$comment
Nitrosobenzene
Nuclear Repulsion Energy = 324.55877006 hartrees
$end

$molecule
0 1
  C   0.5511596405   0.2248256741   0.0000000000
  C  -0.3371075273   1.2975860302  -0.0000000000
  H   0.0642512489   2.3017663857  -0.0000000000
  C  -1.7062315417   1.0492877903  -0.0000000000
  H  -2.4082372231   1.8711445447  -0.0000000000
  C  -2.1690464525  -0.2654631376  -0.0000000000
  H  -3.2325260915  -0.4615222621  -0.0000000000
  C   0.1003132488  -1.0957174106   0.0000000000
  H   0.8220183746  -1.8997675501   0.0000000000
  C  -1.2672666621  -1.3339796605   0.0000000000
  H  -1.6380372156  -2.3496484966   0.0000000000
  N   1.9448731995   0.5932527049  -0.0000000000
  O   2.7184367845  -0.3592471590   0.0000000000
$end
```

```
$comment
Pyridazine
Nuclear Repulsion Energy = 207.83513538 hartrees
$end

$molecule
0 1
  N   0.6690250497  -1.2339460170   0.0000000000
  N  -0.6690049502  -1.2339568257   0.0000000000
  C  -1.3194701179  -0.0638605869   0.0000000000
  H  -2.3977746736  -0.1485733507   0.0000000000
  C   1.3194713948  -0.0638393148  -0.0000000000
  H   2.3977773146  -0.1485347139  -0.0000000000
  C   0.6913452653   1.1793857151  -0.0000000000
  H   1.2680210316   2.0930430490  -0.0000000000
  C  -0.6913647347   1.1793745696   0.0000000000
  H  -1.2680552142   2.0930226167  -0.0000000000
$end


$comment
Acetonitrile
Nuclear Repulsion Energy = 58.25693243 hartrees
$end

$molecule
0 1
  H  -1.5538092910  -0.3739915064   0.9504102102
  C  -1.1827840058   0.0000134229  -0.0000082024
  H  -1.5538509575  -0.6361575946  -0.7990089449
  H  -1.5538977557   1.0100410342  -0.1513307442
  C   0.2748714404   0.0000070652  -0.0000050541
  N   1.4441476281  -0.0000021231   0.0000012882
$end


$comment
Formamide
Nuclear Repulsion Energy = 71.23527648 hartrees
$end

$molecule
0 1
  C   0.1594929240  -0.3873840762   0.0000000000
  H   0.1290681453  -1.4873113711   0.0000000000
  O   1.1971833014   0.2444830106  -0.0000000000
  N  -1.0832689128   0.1591549883  -0.0000000000
  H  -1.9022171056  -0.4171937698   0.0000000000
  H  -1.1783926045   1.1588605951  -0.0000000000
$end
```

```
$comment
N,N-dimethylformamide
Nuclear Repulsion Energy = 181.99836537 hartrees
$end

$molecule
0 1
  N   0.3626792498  -0.0051665302  -0.0000000000
  C  -0.7924569973   0.7001170262   0.0000000000
  H  -0.6231062200   1.7886391109   0.0000000000
  O  -1.9079221267   0.2007953140   0.0000000000
  C   0.2627078342  -1.4537018388  -0.0000000000
  H   1.2620449459  -1.8774312074  -0.0000000000
  H  -0.2769649161  -1.8017725081  -0.8792367504
  H  -0.2769649161  -1.8017725081   0.8792367504
  C   1.6420238931   0.6820226180   0.0000000000
  H   2.4357903957  -0.0581022244   0.0000000000
  H   1.7650872981   1.3048078523  -0.8855274780
  H   1.7650872981   1.3048078523   0.8855274780
$end


$comment
Dimethyl sulfoxide
Nuclear Repulsion Energy = 181.99836537 hartrees
$end

$molecule
0 1
  N   0.3626792498  -0.0051665302  -0.0000000000
  C  -0.7924569973   0.7001170262   0.0000000000
  H  -0.6231062200   1.7886391109   0.0000000000
  O  -1.9079221267   0.2007953140   0.0000000000
  C   0.2627078342  -1.4537018388  -0.0000000000
  H   1.2620449459  -1.8774312074  -0.0000000000
  H  -0.2769649161  -1.8017725081  -0.8792367504
  H  -0.2769649161  -1.8017725081   0.8792367504
  C   1.6420238931   0.6820226180   0.0000000000
  H   2.4357903957  -0.0581022244   0.0000000000
  H   1.7650872981   1.3048078523   0.8855274780
$end
```

```
$comment
Nitromethane
Nuclear Repulsion Energy = 181.99836537 hartrees
$end

$molecule
0 1
  N   0.1688872759   0.0000617577  -0.0099356859
  O   0.7268248224   1.0931786401   0.0027999582
  O   0.7277142040  -1.0927624828   0.0027984852
  C  -1.3146733445  -0.0004913291  -0.0025716396
  H  -1.6515514876  -0.9053007738  -0.4916986564
  H  -1.6516846788   0.8969812189  -0.5049640370
  H  -1.6272469084   0.0075059674   1.0368547847
$end


$comment
Methyl isocyanide
Nuclear Repulsion Energy = 59.94456555 hartrees
$end

$molecule
0 1
  N   0.3087833820  -0.0003091100  -0.0000295292
  C   1.4878422678   0.0002074444   0.0000201182
  C  -1.1114625696   0.0000605312  -0.0000002176
  H  -1.4732799273  -1.0184723733  -0.1015408599
  H  -1.4732451843   0.5974889211  -0.8312434894
  H  -1.4732367514   0.4215393686   0.9328716498
$end


$comment
Vinylene carbonate
Nuclear Repulsion Energy = 229.41686270 hartrees
$end

$molecule
0 1
  O  -1.1096046400  -0.0000000000   0.0219174472
  C   0.0000000000   0.0000000000  -0.7822878971
  O   0.0000000000   0.0000000000  -1.9731658971
  O   1.1096046400   0.0000000000   0.0219174472
  C  -0.6662880114  -0.0000000000   1.3264693103
  H  -1.4026126464  -0.0000000000   2.1053700170
  C   0.6662880114   0.0000000000   1.3264693103
  H   1.4026126464   0.0000000000   2.1053700170
$end
```

```
$comment
Acetone
Nuclear Repulsion Energy = 119.58538797 hartrees
$end

$molecule
0 1
  C   0.0000000026  -0.0000000000   0.1837019532
  O   0.0000000000   0.0000000000   1.4010539532
  C  -1.2809275915  -0.0000000000  -0.6146872465
  H  -2.1343486622  -0.0000000000   0.0553027728
  H  -1.3168579545   0.8766331563  -1.2612506963
  H  -1.3168579545  -0.8766331563  -1.2612506963
  C   1.2809275915   0.0000000000  -0.6146872465
  H   2.1343486622   0.0000000000   0.0553027728
  H   1.3168579545   0.8766331563  -1.2612506963
  H   1.3168579545  -0.8766331563  -1.2612506963
$end
```

```
$comment
Testosterone
Nuclear Repulsion Energy = 1841.15656587 hartrees
$end

$molecule
0 1
  C   0.3151979776   0.3890792254   0.1558941975
  H   0.4436518150   0.2439899000   1.2395279817
  C  -0.4265990478   1.7196224485  -0.0364161056
  H   0.1497602077   2.5301279039   0.4102027289
  H  -0.5067411144   1.9457975721  -1.1006900650
  C  -1.8291243030   1.7101531598   0.5808782757
  H  -2.3248073189   2.6642921264   0.3763653413
  H  -1.7421753099   1.6140666522   1.6688177743
  C  -2.6455490097   0.5419670457   0.0498112993
  C  -2.9653209219   0.7264737673  -1.4329863586
  H  -2.0643413470   0.8094630089  -2.0376635266
  H  -3.5549884803  -0.0999200332  -1.8267380011
  H  -3.5526081323   1.6336962072  -1.5702772496
  C  -1.8819969419  -0.7524941187   0.3424509965
  H  -1.6988411891  -0.7586546912   1.4278843890
  C  -0.5173058558  -0.8146751082  -0.3210990408
  H  -0.6508590271  -0.7657599109  -1.4078897259
  C   0.2020699168  -2.1130716357   0.0173749338
  H  -0.3757391580  -2.9701433307  -0.3332239379
  H   0.2823168918  -2.1983375792   1.1062717297
  C   1.5973841021  -2.1379484032  -0.5985159493
```

```
  H   2.1375217168  -3.0435124234  -0.3204803177
  H   1.4956623492  -2.1484917750  -1.6886987932
  C   2.3960925108  -0.9335661210  -0.1989379431
  C   3.6312961809  -1.0817562131   0.3245266470
  H   4.0299933450  -2.0725798776   0.5091489153
  C   4.5383317957   0.0384905191   0.6057565183
  O   5.6226328874  -0.1276137491   1.1488517251
  C   4.0627787408   1.3836877823   0.1188396298
  H   4.6035212139   2.1603181264   0.6569214417
  H   4.3366174798   1.4659492513  -0.9364248323
  C   1.7570011240   0.4196531840  -0.4321698136
  C   2.5556923784   1.5141469330   0.2926856630
  H   2.2313752561   2.4950287895  -0.0557232396
  H   2.3230824872   1.4588538269   1.3607468110
  C  -2.9073896525  -1.8558598237   0.0516036578
  H  -2.6997097944  -2.7676311484   0.6086693008
  H  -2.8938715409  -2.1146658070  -1.0083623676
  C  -3.9411637083   0.2418198709   0.8158786739
  H  -3.7175127098   0.3154056766   1.8878405856
  O  -5.0582655188   1.0587055707   0.4985259905
  H  -4.8973832328   1.9305729525   0.8732377584
  C  -4.2594641743  -1.2165037817   0.4520225511
  H  -4.7352441476  -1.7333072863   1.2826364733
  H  -4.9695561923  -1.2123322788  -0.3738668578
  C   1.7477563102   0.6974710902  -1.9443972182
  H   1.1313882782  -0.0188649953  -2.4853804019
  H   1.3681398841   1.6971413941  -2.1530731623
  H   2.7582842875   0.6306242515  -2.3480041642
$end



$comment
Progesterone
Nuclear Repulsion Energy = 2083.85428949 hartrees
$end

$molecule
0 1
  C  -0.7797679261   0.3189572245  -0.1038775534
  H  -0.8740735065   0.2070288510  -1.1949677612
  C   0.0405559578   1.5911521430   0.1497173240
  H  -0.4659133318   2.4498973505  -0.2913373647
  H   0.0992427734   1.7843094249   1.2221520936
  C   1.4593825386   1.5113393380  -0.4226706090
  H   2.0152308124   2.4189683278  -0.1830989520
  H   1.4023927828   1.4403756044  -1.5147114188
  C   2.1843433554   0.2831366870   0.1085368993
```

```
  C   2.4380862697   0.4051764584   1.6147484753
  H   2.9961334851   1.3161445677   1.8195942866
  H   1.5083365867   0.4396523178   2.1792334083
  H   3.0173321191  -0.4357134667   1.9966817059
  C   3.4802329703  -0.0900079856  -0.6210758196
  H   3.2761902323  -0.0303782314  -1.6993542570
  C   4.6913364274   0.7887883183  -0.4089357982
  O   4.6254966616   1.8807460613   0.1316226320
  C   5.9996162376   0.2556040590  -0.9444092485
  H   6.7503067810   1.0395370693  -0.9217872687
  H   5.8748566161  -0.1210674930  -1.9593089789
  H   6.3325924059  -0.5813901450  -0.3301902574
  C   1.3445657127  -0.9557415504  -0.2380548274
  H   1.2021434172  -0.9241882608  -1.3287660901
  C  -0.0456447377  -0.9467845379   0.3735628692
  H   0.0466073523  -0.9336205162   1.4652087275
  C  -0.8318893780  -2.1883484779  -0.0257453071
  H  -0.3261726198  -3.0897179424   0.3255230964
  H  -0.8733696710  -2.2434047569  -1.1187657590
  C  -2.2498832916  -2.1362814052   0.5345772441
  H  -2.8347958420  -2.9989050995   0.2138038398
  H  -2.1927366185  -2.1773468215   1.6272795963
  C  -2.9529504151  -0.8738958082   0.1347150712
  C  -4.1709332662  -0.9295210319  -0.4440374128
  H  -4.6240619526  -1.8877033716  -0.6707678935
  C  -4.9907539999   0.2540800909  -0.7340985657
  O  -6.0558746581   0.1725607833  -1.3318408548
  C  -4.4539877920   1.5517420973  -0.1864869339
  H  -4.9227206621   2.3768661644  -0.7197590051
  H  -4.7649110708   1.6194083660   0.8595487445
  C  -2.2386147168   0.4286838858   0.4291734825
  C  -2.9355421482   1.5906581945  -0.2956800043
  H  -2.5648708770   2.5391158848   0.0934846392
  H  -2.6618144671   1.5487882684  -1.3545421410
  C   2.2787612271  -2.1307678456   0.0645145067
  H   2.0349961032  -3.0158391872  -0.5206175940
  H   2.2077462621  -2.4086415831   1.1173345043
  C  -2.2711456516   0.6689045847   1.9474175768
  H  -1.7244156284  -0.0990423325   2.4925017121
  H  -1.8350635840   1.6358227131   2.1958795299
  H  -3.2989068406   0.6595409937   2.3109912659
  C   3.6926093581  -1.5870750860  -0.2673860222
  H   4.1572286990  -2.1291501291  -1.0892191433
  H   4.3552538271  -1.6845974402   0.5926904339
$end
```

```
$comment
Cortisol
Nuclear Repulsion Energy = 2633.34219375 hartrees
$end

$molecule
0 1
  O   0.3156478415  -2.0698068978   1.1898150821
  H  -0.2777404043  -2.8289344911   1.1604299270
  C   0.3260442414  -1.5031905472  -0.1261591021
  H   0.8407073745  -2.1969660347  -0.7980803395
  C  -1.0932453888  -1.3222686617  -0.6782135396
  H  -1.0292384747  -1.1566473619  -1.7542593176
  H  -1.6481437889  -2.2554820086  -0.5394409558
  C  -1.8227711057  -0.1439801562  -0.0506686867
  C  -2.1673910296  -0.4003645381   1.4188275627
  H  -1.2740236844  -0.6481707080   1.9827967859
  H  -2.6252372036   0.4721286071   1.8862855389
  H  -2.8607010752  -1.2372724331   1.5128163821
  C  -0.9583506330   1.1089666423  -0.2245068858
  H  -0.7434638906   1.1816499669  -1.2958898661
  C   0.3873061026   1.0113880761   0.4743728674
  H   0.2413730239   0.8927349828   1.5525315210
  C   1.1917300396   2.2813119205   0.2082484690
  H   0.6970538008   3.1426769662   0.6614245379
  H   1.2086197099   2.4516898345  -0.8736043102
  C   2.6249505022   2.1785524513   0.7189265474
  H   3.2024181222   3.0603006048   0.4387187434
  H   2.6084331525   2.1417757751   1.8126107393
  C   3.3085290651   0.9436263128   0.2150422666
  C   4.5217794421   1.0163552569  -0.3703309746
  H   4.9861556486   1.9792442788  -0.5496451587
  C   5.3270525291  -0.1633135568  -0.7162989085
  O   6.3829705984  -0.0692518888  -1.3284950133
  C   4.7905569085  -1.4749220504  -0.2002946164
  H   5.2566493958  -2.2863431121  -0.7563336195
  H   5.1004099972  -1.5698222567   0.8437827233
  C   2.5870326508  -0.3652842006   0.4577061962
  C   3.2720115593  -1.5042738296  -0.3095986721
  H   2.8869581459  -2.4593623691   0.0498347952
  H   3.0043370354  -1.4213198477  -1.3679256660
  C  -1.9013552581   2.2635639011   0.1319549510
  H  -1.6402845212   3.1810198594  -0.3914285298
  H  -1.8605486894   2.4794093101   1.2008022985
  C   1.1401773536  -0.2001596684  -0.1029474401
  H   1.2819701931   0.0405540674  -1.1678938474
```

```
  C    2.6484431604  -0.6372677575   1.9734970887
  H    2.2985777979  -1.6385996000   2.2006544886
  H    2.0332299583   0.0640835512   2.5342683164
  H    3.6754612680  -0.5240564962   2.3236209778
  C   -3.0974104727   0.3159837780  -0.8012197771
  O   -2.7411494626   0.3746719394  -2.1858879942
  H   -3.5358179483   0.5842283500  -2.6893916160
  C   -4.2662004302  -0.6693335310  -0.6544116991
  O   -4.1904651408  -1.7619496665  -1.1912886780
  C   -5.5369769259  -0.2824356846   0.0990007944
  H   -6.2850487164  -1.0296007456  -0.1492289811
  H   -5.8865281021   0.6985308524  -0.2375023499
  O   -5.3867521861  -0.3302150786   1.5105062943
  H   -4.7797244254   0.3663834084   1.7760140236
  C   -3.3097017649   1.7510515919  -0.2712077835
  H   -3.9896065240   1.7833638422   0.5795861993
  H   -3.7615236544   2.3611814534  -1.0530629146
$end
```

1.3 Excite dipole-bound states of closed-shell anions

```
$comment
Cyanomethyl anion
Nuclear Repulsion Energy = 52.35839501 hartrees
$end

$molecule
-1 1
   C  -0.1795589102   0.0017252380  -0.0000000000
   N  -1.3702124120   0.0127993379  -0.0000000000
   C   1.2152986273  -0.1033284197   0.0000000000
   H   1.6885242909   0.2600118626   0.9078030521
   H   1.6885242909   0.2600118626  -0.9078030521
$end


   $comment
   9-Anthroxide
   Nuclear Repulsion Energy = 869.94286791 hartrees
   $end

   $molecule
   -1 1
      O   0.0000000000   0.0000000000   2.5558359048
      C   0.0000000000   0.0000000000   1.2992249048
      C   0.0000000000   0.0000000000  -1.6232905048
      C   1.2114124089   0.0000000000  -0.9210087580
      C  -1.2114124089  -0.0000000000  -0.9210087580
      C   1.2287628180   0.0000000000   0.5143780476
      C  -1.2287628226  -0.0000000000   0.5143780499
      C   2.4642472785   0.0000000000   1.1949586597
      C  -2.4642472785  -0.0000000000   1.1949586597
      C   2.4696442069   0.0000000000  -1.5882299661
      C  -2.4696442069  -0.0000000000  -1.5882299661
      C   3.6631268536   0.0000000000   0.5146921362
      C  -3.6631268536  -0.0000000000   0.5146921362
      C   3.6615792470   0.0000000000  -0.8999980173
      C  -3.6615792470  -0.0000000000  -0.8999980173
      H   0.0000000000   0.0000000000  -2.7080985048
      H   2.4209840238   0.0000000000   2.2769480620
      H  -2.4209840253  -0.0000000000   2.2769480664
      H   2.4735165418   0.0000000000  -2.6738730600
      H  -2.4735165418  -0.0000000000  -2.6738730600
      H   4.5985990543   0.0000000000  -1.4451401679
      H  -4.5985990543  -0.0000000000  -1.4451401679
      H   4.6011091968   0.0000000000   1.0562150609
      H  -4.6011091968  -0.0000000000   1.0562150609
   $end
```

```
$comment
2-Naphthoxide
Nuclear Repulsion Energy = 530.42332952 hartrees
$end

$molecule
-1 1
   O  -3.4299176974  -0.6970275445   0.0000000000
   C   0.2326459785  -0.6330027032  -0.0000000000
   C   0.4826882869   0.7850131822  -0.0000000000
   C  -0.6460798238   1.6431206839  -0.0000000000
   C  -1.0802474995  -1.1227004370   0.0000000000
   C   1.3727091509  -1.4855578130  -0.0000000000
   C   1.8071069360   1.2663222522  -0.0000000000
   C  -1.9221392888   1.1387460522   0.0000000000
   C  -2.2354796674  -0.2855571954   0.0000000000
   C   2.6599950275  -0.9879982069  -0.0000000000
   C   2.8891880944   0.4051498662  -0.0000000000
   H  -0.4822845801   2.7176655355  -0.0000000000
   H   1.2104015764  -2.5587749385   0.0000000000
   H  -1.2417731420  -2.1965209288   0.0000000000
   H   1.9642680458   2.3410590280  -0.0000000000
   H  -2.7737978598   1.8116817667   0.0000000000
   H   3.5000440089  -1.6733219080  -0.0000000000
   H   3.9001603625   0.7932177137  -0.0000000000
$end


$comment
Phenoxide
Nuclear Repulsion Energy = 259.68466743 hartrees
$end

$molecule
-1 1
   O   0.0000000000   0.0000000000   2.3499026609
   C   0.0000000000   0.0000000000   1.0827496609
   C   0.0000000000   0.0000000000  -1.8285590810
   C   1.1967659112  -0.0000000000  -1.1029502085
   C  -1.1967659112   0.0000000000  -1.1029502085
   C   1.2025959940  -0.0000000000   0.2865025602
   C  -1.2025959940   0.0000000000   0.2865025602
   H   0.0000000000   0.0000000000  -2.9111380810
   H   2.1441220426  -0.0000000000   0.8263378633
   H  -2.1441220426   0.0000000000   0.8263378633
   H   2.1449121067  -0.0000000000  -1.6342660221
   H  -2.1449121067   0.0000000000  -1.6342660221
$end
```

1.4 Quadrupole-bound anions

```
$comment
Terephthalonitrile
Nuclear Repulsion Energy = 406.56399256 hartrees
$end

$molecule
0 1
  H   1.2422296847   2.1457578212   0.0000000000
  H   1.2422296848  -2.1457578212  -0.0000000000
  H  -1.2422296848   2.1457578211   0.0000000000
  H  -1.2422296848  -2.1457578212  -0.0000000000
  C   0.6935312672   1.2148881997   0.0000000000
  C   0.6935312672  -1.2148881997  -0.0000000000
  C  -0.6935312673   1.2148881996   0.0000000000
  C  -0.6935312672  -1.2148881997  -0.0000000000
  C   1.3898130926   0.0000000000   0.0000000000
  C  -1.3898130926  -0.0000000001  -0.0000000000
  C   2.8195237224   0.0000000000   0.0000000000
  C  -2.8195237224   0.0000000001   0.0000000000
  N   3.9930935740   0.0000000001   0.0000000000
  N  -3.9930935738   0.0000000000   0.0000000000
$end
```

```
$comment
p-Diisocyanobenzene
Nuclear Repulsion Energy = 415.42632682 hartrees
$end

$molecule
0 1
  H   1.2498365677   2.1414942565  -0.0000000000
  H   1.2498365677  -2.1414942567   0.0000000000
  H  -1.2498365677   2.1414942567  -0.0000000000
  H  -1.2498365677  -2.1414942567   0.0000000000
  C   0.6937576123   1.2155637444  -0.0000000000
  C   0.6937576124  -1.2155637446   0.0000000000
  C  -0.6937576123   1.2155637445  -0.0000000000
  C  -0.6937576123  -1.2155637446   0.0000000000
  C   1.3796157636  -0.0000000000   0.0000000000
  C  -1.3796157636  -0.0000000000   0.0000000000
  N   2.7603928025   0.0000000001  -0.0000000000
  N  -2.7603928025   0.0000000001  -0.0000000000
  C   3.9450306333   0.0000000001  -0.0000000000
  C  -3.9450306334   0.0000000001  -0.0000000000
$end
```

```
$comment
Succinonitrile
Nuclear Repulsion Energy = 178.87883005 hartrees
$end

$molecule
0 1
  C   0.4712426054  -0.6068960308  -0.0000012082
  C  -0.4712426054   0.6068960308   0.0000000000
  H   0.2890669612  -1.2235512733   0.8786880203
  H   0.2890669612  -1.2235512733  -0.8786880203
  H  -0.2890669612   1.2235512733   0.8786880203
  H  -0.2890669612   1.2235512733  -0.8786880203
  C   1.8642109231  -0.1726011128  -0.0000004321
  C  -1.8642109231   0.1726011128   0.0000000000
  N   2.9704602178   0.2093874155   0.0000017738
  N  -2.9704602178  -0.2093874155   0.0000000000
$end


$comment
2,6-Dicyanonaphthalene
Nuclear Repulsion Energy = 709.54831541 hartrees
$end

$molecule
0 1
  C   0.2205566662   0.6804087650   0.0000000000
  C  -0.2205566662  -0.6804087650   0.0000000000
  C   0.7423460633  -1.7180049284  -0.0000000000
  C  -0.7423460633   1.7180049284  -0.0000000000
  C   1.6030858003   0.9550288811   0.0000000000
  C  -1.6030857986  -0.9550288837  -0.0000000000
  C   2.0857483054  -1.4310483373  -0.0000000000
  C  -2.0857483054   1.4310483373  -0.0000000000
  C   2.5196119567  -0.0819472718  -0.0000000000
  C  -2.5196119567   0.0819472718  -0.0000000000
  H   0.4062995313  -2.7469465879  -0.0000000000
  H  -0.4062995313   2.7469465879  -0.0000000000
  H   1.9479970191   1.9810456666  -0.0000000000
  H  -1.9479970191  -1.9810456666  -0.0000000000
  H   2.8214860020  -2.2227753429  -0.0000000000
  H  -2.8214860020   2.2227753429  -0.0000000000
  C   3.9200097805   0.2053787857   0.0000000000
  C  -3.9200097805  -0.2053787857   0.0000000000
  N   5.0712512565   0.4341409472   0.0000000000
  N  -5.0712512565  -0.4341409472   0.0000000000
$end
```

```
$comment
p-Dinitrobenzene
Nuclear Repulsion Energy = 660.96984418 hartrees
$end
$molecule
0 1
  C   1.3615906780   0.0000000000  -0.0000000000
  C  -1.3615906780  -0.0000000000  -0.0000000000
  C   0.6944778617   1.2191745904  -0.0000000000
  C   0.6944778617  -1.2191745903   0.0000000000
  C  -0.6944778618   1.2191745904  -0.0000000000
  C  -0.6944778617  -1.2191745903   0.0000000000
  H   1.2605803387   2.1371547091  -0.0000000000
  H  -1.2605803387   2.1371547091  -0.0000000000
  H   1.2605803387  -2.1371547091   0.0000000000
  H  -1.2605803387  -2.1371547090   0.0000000000
  N   2.8321219727   0.0000000000  -0.0000000000
  N  -2.8321219727  -0.0000000000   0.0000000000
  O   3.3947244689   1.0920129331  -0.0000000000
  O   3.3947244689  -1.0920129332   0.0000000000
  O  -3.3947244689   1.0920129331  -0.0000000000
  O  -3.3947244688  -1.0920129332   0.0000000000
$end

$comment
Tetracyanobenzene
Nuclear Repulsion Energy = 676.34160238 hartrees
$end
$molecule
0 1
  C   0.0000000000   1.4002263649   0.0000000000
  C   0.0000000485  -1.4002263649   0.0000000000
  H   0.0000000000   2.4810183649   0.0000000000
  H   0.0000001373  -2.4810183649   0.0000000000
  C   1.2091675824   0.7046656395   0.0000000000
  C   1.2091675824  -0.7046656395  -0.0000000000
  C  -1.2091675824   0.7046656395  -0.0000000000
  C  -1.2091675824  -0.7046656395   0.0000000000
  C   2.4412737175   1.4244734446  -0.0000000000
  C   2.4412737175  -1.4244734446   0.0000000000
  C  -2.4412737175   1.4244734446   0.0000000000
  C  -2.4412737175  -1.4244734446  -0.0000000000
  N   3.4479648091   2.0293108905  -0.0000000000
  N   3.4479648091  -2.0293108905   0.0000000000
  N  -3.4479648091   2.0293108905   0.0000000000
  N  -3.4479648091  -2.0293108905  -0.0000000000
$end
```

```
$comment
sym-Tetracyanonaphthalene
Nuclear Repulsion Energy = 1020.25046534 hartrees
$end

$molecule
0 1
  C   0.0000000000   0.7153119208   0.0000000000
  C   0.0000000000  -0.7153119208  -0.0000000000
  C   1.2294867825   1.4056580791   0.0000000000
  C   1.2294867825  -1.4056580791  -0.0000000000
  C  -1.2294867825   1.4056580791   0.0000000000
  C  -1.2294867825  -1.4056580791  -0.0000000000
  H   1.2402503710   2.4878776537   0.0000000000
  H   1.2402503710  -2.4878776537  -0.0000000000
  H  -1.2402503710   2.4878776537   0.0000000000
  H  -1.2402503710  -2.4878776537  -0.0000000000
  C   2.4254112789   0.7126552134   0.0000000000
  C   2.4254112789  -0.7126552134  -0.0000000000
  C  -2.4254112789   0.7126552134   0.0000000000
  C  -2.4254112789  -0.7126552134  -0.0000000000
  C   3.6627422331   1.4244689355   0.0000000000
  C   3.6627422331  -1.4244689355  -0.0000000000
  C  -3.6627422331   1.4244689355   0.0000000000
  C  -3.6627422331  -1.4244689355  -0.0000000000
  N   4.6734053815   2.0224932683   0.0000000000
  N   4.6734053815  -2.0224932683  -0.0000000000
  N  -4.6734053815   2.0224932683   0.0000000000
  N  -4.6734053815  -2.0224932683  -0.0000000000
$end
```

1.5 Correlation-bound anions

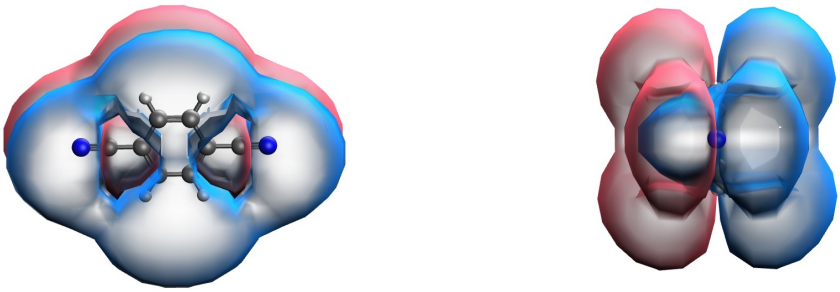
```
$comment
Hexafluorobenzene
Nuclear Repulsion Energy = 734.40650321 hartrees
$end

$molecule
0 1
  C   1.3697013386   0.2355844032  -0.0000000000
  C  -1.3697013386  -0.2355844032  -0.0000000000
  C   0.8888796645  -1.0684122879  -0.0000000000
  C  -0.8888796645   1.0684122879  -0.0000000000
  C   0.4808286423   1.3039941574   0.0000000000
  C  -0.4808286423  -1.3039941574   0.0000000000
  F   0.9403848257   2.5502759181   0.0000000000
  F  -0.9403848257  -2.5502759181   0.0000000000
  F   1.7384186974  -2.0895320529  -0.0000000000
  F  -1.7384186974   2.0895320529  -0.0000000000
  F  -2.6787934184  -0.4607480456   0.0000000000
  F   2.6787934184   0.4607480456   0.0000000000
$end
```

```
$comment
Perfluorocubane
Nuclear Repulsion Energy = 1284.52287119 hartrees
$end

$molecule
0 1
  C   0.7863625069   0.7863625055   0.7863625027
  C   0.7863625069   0.7863625055  -0.7863625027
  C   0.7863625069  -0.7863625055   0.7863625027
  C   0.7863625069  -0.7863625055  -0.7863625027
  C  -0.7863625069   0.7863625055   0.7863625027
  C  -0.7863625069   0.7863625055  -0.7863625027
  C  -0.7863625069  -0.7863625055   0.7863625027
  C  -0.7863625069  -0.7863625055  -0.7863625027
  F   1.5568185472   1.5568185392   1.5568185378
  F   1.5568185472   1.5568185392  -1.5568185378
  F   1.5568185472  -1.5568185392   1.5568185378
  F   1.5568185472  -1.5568185392  -1.5568185378
  F  -1.5568185472   1.5568185392   1.5568185378
  F  -1.5568185472   1.5568185392  -1.5568185378
  F  -1.5568185472  -1.5568185392   1.5568185378
  F  -1.5568185472  -1.5568185392  -1.5568185378
$end
```

```
$comment
Hexachlorobenzene
Nuclear Repulsion Energy = 1349.91415449 hartrees
$end

$molecule
0 1
  C   1.4013140976   0.0000000001   0.0000000000
  C  -1.4013140976  -0.0000000001  -0.0000000000
  C   0.7006574999   1.2135737551  -0.0000000000
  C   0.7006575001  -1.2135737550   0.0000000000
  C  -0.7006574999  -1.2135737551   0.0000000000
  C  -0.7006575001   1.2135737550  -0.0000000000
 Cl  -3.1139980976  -0.0000000001   0.0000000000
 Cl   3.1139980976   0.0000000001   0.0000000000
 Cl  -1.5570060575  -2.6967989764   0.0000000000
 Cl   1.5570060577  -2.6967989763   0.0000000000
 Cl   1.5570060575   2.6967989764  -0.0000000000
 Cl  -1.5570060577   2.6967989763  -0.0000000000
$end


$comment
Octafluoronaphthalene
Nuclear Repulsion Energy = 1385.99890539 hartrees
$end

$molecule
0 1
  C   2.4241213154   0.7015895000   0.0000000000
  C   2.4241213154  -0.7015895000   0.0000000000
  C  -2.4241213154  -0.7015895000   0.0000000000
  C  -2.4241213154   0.7015895000   0.0000000000
  C   1.2385377850  -1.3968651896   0.0000000000
  C   1.2385377850   1.3968651896   0.0000000000
  C  -1.2385377850   1.3968651896  -0.0000000000
  C  -1.2385377850  -1.3968651896  -0.0000000000
  C   0.0000000000   0.7193030502   0.0000000000
  C   0.0000000000  -0.7193030502   0.0000000000
  F   1.2907397534   2.7265138603  -0.0000000000
  F   1.2907397534  -2.7265138603  -0.0000000000
  F  -1.2907397534   2.7265138603   0.0000000000
  F  -1.2907397534  -2.7265138603  -0.0000000000
  F   3.5850705108  -1.3442887067  -0.0000000000
  F   3.5850705108   1.3442887067  -0.0000000000
  F  -3.5850705108   1.3442887067   0.0000000000
  F  -3.5850705108  -1.3442887067   0.0000000000
$end
```

2 EOMEA-CCSD Dyson orbitals of valence anions

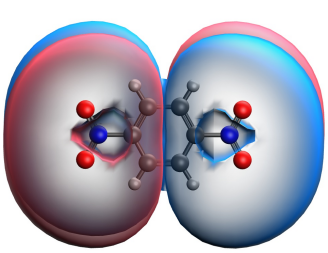
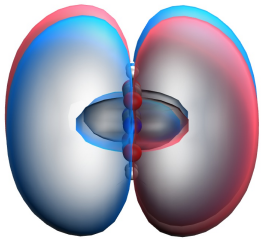
Terephthalonitrile (B_{1u} state)



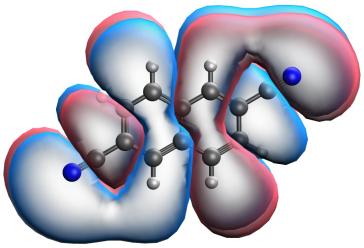
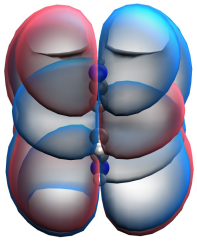
p-Diisocyanobenzene (B_{1u} state)

p-Dinitrobenzene (B_{1u} state)

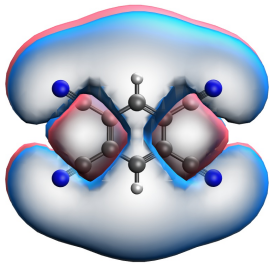
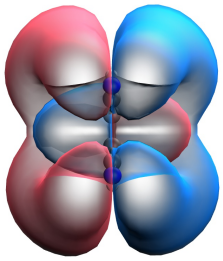
p-Dinitrobenzene (B_{2g} state)

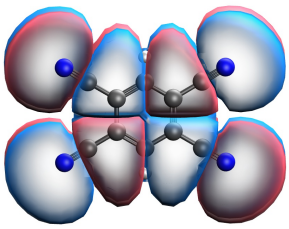
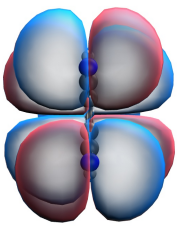
2,6-Dicyanonaphthalene (B_g state)

Tetracyanobenzene (B_{1u} state)

Tetracyanobenzene (A_u state)

3 Basis-set orthogonalization

		Number of basis functions	Number of orthogonal orbitals	% retained
Dipole-bound radical anions				
Acetonitrile	CH_3CN	261	256	98.1
Formamide	CH_3NO	261	256	98.1
Methyl isocyanide	CH_3NC	261	256	98.1
Nitromethane	CH_3NO_2	322	317	98.4
Acetone	$(CH_3)_2CO$	400	390	97.5
Dimethyl sulfoxide	$(CH_3)_2SO$	404	397	98.3
Vinylene carbonate	$C_3H_2O_3$	418	401	95.9
Pyridazine	$C_4H_4N_2$	470	446	94.9
N,N-Dimethylformamide	$(CH_3)_2NCHO$	487	470	96.5
Uracil	$C_4H_4N_2O_2$	592	557	94.1
Benzonitrile	C_6H_5CN	618	576	93.2
Phenyl isocyanide	C_6H_5NC	618	577	93.4
Nitrosobenzene	C_6H_5NO	618	579	93.7
Benzaldehyde	C_6H_5CHO	644	600	93.2
Nitrobenzene	$C_6H_5NO_2$	679	634	93.4
Testosterone	$C_{19}H_{28}O_2$	2009	1762	87.7
Progesterone	$C_{21}H_{30}O_2$	2183	1908	87.4
Cortisol	$C_{21}H_{30}O_5$	2366	2058	87.0
Excited dipole-bound states of closed shell anions				
Cyanomethyl anion	CH_2CN^-	235	231	98.3
Phenoxide	$C_6H_5O^-$	557	524	94.1
2-Naphthoxide	$C_{10}H_7O^-$	853	775	90.9
9-Anthroxide	$C_{14}H_9O^-$	1149	1020	88.8
Quadrupole-bound anions				
Succinonitrile	$C_4H_4N_2$	470	452	96.2
Terephthalonitrile	$C_6H_4(CN)_2$	714	658	92.2
p-Diisocyanobenzene	$C_6H_4(NC)_2$	714	660	92.4
p-Dinitrobenzene	$C_6H_4(NO_2)_2$	836	774	92.6
Tetracyanobenzene	$C_6H_2(CN)_4$	906	820	90.5
2,6-Dicyanonaphthalene	$C_{10}H_6(CN)_2$	1010	907	89.8
sym-Tetracyanonaphthalene	$C_{10}H_4(CN)_4$	1202	1068	88.9
Correlation-bound anions				
Hexafluorobenzene	C_6F_6	888	738	83.1
Hexachlorobenzene	C_6Cl_6	912	769	84.3
Octafluorocubane	C_8F_8	1184	947	80.0
Octafluoronaphthalene	$C_{10}F_8$	1332	1058	79.4