Supplementary Material for "Electrostatic Potential and a Simple Extended Electric Dipole Model of Hydrogen Fluoride as Probes of Non-Bonding Electron Pairs in the Cyclic Ethers 2,5-Dihydrofuran, Oxetane and Oxirane"

Optimised geometries of the cyclic ethers

Oxirane

7
CCSD(T)-F12C/VTZ-F12 ENERGY=-153.60887101

C	0.7316902300	-0.0000000000	-0.4263516266
O	-0.0000000000	-0.0000000000	0.8005887807
C	-0.7316902300	0.0000000000	-0.4263516266
H	1.2627161143	0.9196408327	-0.6404724583
H	1.2627161143	-0.9196408327	-0.6404724583
H	-1.2627161143	-0.9196408327	-0.6404724583
H	-1.2627161143	0.9196408327	-0.6404724583

Oxetane

10
CCSD(T)-F12C/VTZ-F12 ENERGY=-192.86720438

C	1.0362428207	-0.0000000000	0.0608877412
H	1.6618148367	0.8914779030	0.1315607522
H	1.6618148367	-0.8914779030	0.1315607522
C	-0.0000000000	-0.0000000000	-1.0758629972
H	-0.0000000000	-0.8887725598	-1.7016952524
H	-0.0000000000	0.8887725598	-1.7016952524
C	-1.0362428207	-0.0000000000	0.0608877412
H	-1.6618148367	-0.8914779030	0.1315607522
H	-1.6618148367	0.8914779030	0.1315607522
O	-0.0000000000	-0.0000000000	1.0672910106

2,5-dihydrofuran

11
CCSD(T)-F12C/VTZ-F12 ENERGY=-230.92306597

O	0.0000000000	0.0000000000	1.1651007080
C	1.1717725739	0.0000000000	0.3504911823
C	-1.1717725739	0.0000000000	0.3504911823
C	0.6655016103	0.0000000000	-1.0615960339
C	-0.6655016103	0.0000000000	-1.0615960339
H	1.3108436359	0.0000000000	-1.9280277373
H	-1.3108436359	0.0000000000	-1.9280277373
H	1.7740576181	0.8861199552	0.5771569622
H	1.7740576181	-0.8861199552	0.5771569622
H	-1.7740576181	-0.8861199552	0.5771569622
H	-1.7740576181	0.8861199552	0.5771569622

Optimised geometries of the cyclic ether…HF complexes

Oxirane…HF

9
CCSD(T)-F12C/VTZ-F12 ENERGY=-254.01244272

O	0.8847284714	0.0000000000	-0.7336270110
C	1.5147937621	-0.7310086985	0.3362717824
C	1.5147937621	0.7310086985	0.3362717824
H	2.4061577271	1.2650143990	0.0360725434
H	0.8233900674	1.2572469314	0.9818369302
H	0.8233900674	-1.2572469314	0.9818369302

```
H        2.4061577271      -1.2650143990       0.0360725434
H       -0.7550859128       0.0000000000      -0.4566357198
F       -1.6214656717       0.0000000000      -0.0926657809
```

Oxetane…HF

```
 12
CCSD(T)-F12C/VTZ-F12  ENERGY=-293.27309371
C        1.0397523067      -0.0615081985      -0.1081806268
O        0.0000000000      -0.1498259346       0.9083592398
C       -1.0397523067      -0.0615081985      -0.1081806268
C        0.0000000000       0.2493616246      -1.1950370863
H        1.7557580134       0.7212565990       0.1343865049
H        1.5498882803      -1.0191215071      -0.2192811715
H        0.0000000000      -0.4081760834      -2.0596502773
H        0.0000000000       1.2871026429      -1.5178600736
H       -1.5498882803      -1.0191215071      -0.2192811715
H       -1.7557580134       0.7212565990       0.1343865049
H        0.0000000000      -1.5858961147       1.6613697691
F        0.0000000000      -2.4818199215       1.9596090150
```

2,5-dihydrofuran…HF

```
 13
CCSD(T)-F12C/VTZ-F12  ENERGY=-331.32797127
O       -0.6863151630      -0.3917797106       0.0000000000
C       -0.7810695175       0.4221015132       1.1826060574
C       -0.7810695175       0.4221015132      -1.1826060574
C       -0.9242995872       1.8203874108       0.6653219898
C       -0.9242995872       1.8203874108      -0.6653219898
H        0.1216485700       0.2806394626       1.7832779312
H       -1.6444323865       0.0962957031       1.7685242385
H       -1.6444323865       0.0962957031      -1.7685242385
H        0.1216485700       0.2806394626      -1.7832779312
H       -1.0140252556       2.6824661162       1.3094772177
H       -1.0140252556       2.6824661162      -1.3094772177
H        0.6474881242      -1.3297949052       0.0000000000
F        1.4708743919      -1.7874107961       0.0000000000
```

Distributed multipole analyses

The following DMAs have been calculated from CCSD/cc-pV5Z densities using CCSD(T)-F12c/cc-pVTZ-F12 optimised geometries.

Oxirane

```
Distributed multipoles for site   1 ( C) at   1.38269  0.00000 -0.80569
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l        0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.28435E+00   0.30083E+00   0.38314E+00  -0.12819E+01  -0.40970E+00
Ql1c                  -0.24264E-01  -0.44919E+00   0.63686E+00  -0.21398E+00
Ql1s                   0.20431E-14  -0.10999E-15  -0.25140E-15   0.66303E-15
Ql2c                                 0.81983E-01   0.22022E+00  -0.56728E-01
Ql2s                                -0.87230E-16  -0.52046E-15  -0.43940E-15
Ql3c                                              0.12783E+01  -0.15227E+01
Ql3s                                              0.27631E-15   0.51204E-15
Ql4c                                                           0.14349E+01
Ql4s                                                          -0.13159E-14
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.28435E+00   0.30181E+00   0.59606E+00   0.19317E+01   0.21435E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   2 ( C) at  -1.38269  0.00000 -0.80569
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l        0          1          2          3          4
```

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.28435E+00   0.30083E+00   0.38314E+00  -0.12819E+01  -0.40970E+00
Ql1c                0.24264E-01   0.44919E+00  -0.63686E+00   0.21398E+00
Ql1s                0.20005E-14   0.14308E-15  -0.26333E-16  -0.28145E-16
Ql2c                          0.81983E-01   0.22022E+00  -0.56728E-01
Ql2s                         -0.16334E-15   0.25321E-15   0.35269E-15
Ql3c                                   -0.12783E+01   0.15227E+01
Ql3s                                    0.15175E-15   0.17509E-15
Ql4c                                             0.14349E+01
Ql4s                                             0.67825E-15
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.28435E+00   0.30181E+00   0.59606E+00   0.19317E+01   0.21435E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   3 ( O) at   0.00000  0.00000  1.51289
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.39469E+00  -0.33894E+00   0.77534E+00  -0.91097E+00   0.10218E+01
Ql1c                0.20471E-14   0.16735E-14   0.11142E-14  -0.32241E-14
Ql1s                0.34638E-14  -0.53678E-16   0.72761E-16  -0.19546E-15
Ql2c                          0.37265E+00   0.55398E+00  -0.28293E+00
Ql2s                         -0.13991E-15  -0.16342E-15   0.28086E-15
Ql3c                                    0.14522E-15   0.27397E-15
Ql3s                                   -0.54619E-16   0.26684E-15
Ql4c                                             -0.65055E+00
Ql4s                                              0.34481E-16
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.39469E+00   0.33894E+00   0.86024E+00   0.10662E+01   0.12439E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Distributed multipoles for site   4  ( H) at   2.38619  1.73787 -1.21032
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.43505E-01  -0.50879E-01   0.53662E-02   0.65999E-02   0.61408E-01
Ql1c                0.11611E+00   0.10120E-01   0.11574E-01   0.40604E-02
Ql1s                0.18669E+00   0.38031E-01   0.66468E-01   0.22788E-01
Ql2c                         -0.20054E-02   0.12471E-01   0.11223E+00
Ql2s                         -0.32681E-01  -0.44439E-02  -0.77047E-01
Ql3c                                    0.73076E-01   0.24112E-01
Ql3s                                    0.34220E-01   0.55327E-03
Ql4c                                             -0.51113E-01
Ql4s                                             -0.15091E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.43505E-01   0.22566E+00   0.51474E-01   0.10622E+00   0.22092E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   5 ( H) at   2.38619 -1.73787 -1.21032
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.43505E-01  -0.50879E-01   0.53662E-02   0.65999E-02   0.61408E-01
Ql1c                0.11611E+00   0.10120E-01   0.11574E-01   0.40604E-02
Ql1s               -0.18669E+00  -0.38031E-01  -0.66468E-01  -0.22788E-01
Ql2c                         -0.20054E-02   0.12471E-01   0.11223E+00
Ql2s                          0.32681E-01   0.44439E-02   0.77047E-01
Ql3c                                    0.73076E-01   0.24112E-01
Ql3s                                   -0.34220E-01  -0.55327E-03
Ql4c                                             -0.51113E-01
Ql4s                                              0.15091E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.43505E-01   0.22566E+00   0.51474E-01   0.10622E+00   0.22092E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   6 ( H) at  -2.38619 -1.73787 -1.21032
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
Ql0     -0.43505E-01  -0.50879E-01   0.53662E-02   0.65999E-02   0.61408E-01
Ql1c              -0.11611E+00  -0.10120E-01  -0.11574E-01  -0.40604E-02
Ql1s              -0.18669E+00  -0.38031E-01  -0.66468E-01  -0.22788E-01
Ql2c                        -0.20054E-02   0.12471E-01   0.11223E+00
Ql2s                        -0.32681E-01  -0.44439E-02  -0.77047E-01
Ql3c                                  -0.73076E-01  -0.24112E-01
Ql3s                                  -0.34220E-01  -0.55327E-03
Ql4c                                            -0.51113E-01
Ql4s                                            -0.15091E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.43505E-01   0.22566E+00   0.51474E-01   0.10622E+00   0.22092E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

Distributed multipoles for site 7 (H) at -2.38619 1.73787 -1.21032

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.43505E-01  -0.50879E-01   0.53662E-02   0.65999E-02   0.61408E-01
Ql1c              -0.11611E+00  -0.10120E-01  -0.11574E-01  -0.40604E-02
Ql1s               0.18669E+00   0.38031E-01   0.66468E-01   0.22788E-01
Ql2c                        -0.20054E-02   0.12471E-01   0.11223E+00
Ql2s                         0.32681E-01   0.44439E-02   0.77047E-01
Ql3c                                  -0.73076E-01  -0.24112E-01
Ql3s                                   0.34220E-01   0.55327E-03
Ql4c                                            -0.51113E-01
Ql4s                                             0.15091E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.43505E-01   0.22566E+00   0.51474E-01   0.10622E+00   0.22092E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

Total multipoles at the origin

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.11413E-12  -0.78549E+00  -0.28528E+01   0.43307E+01  -0.16622E+01
Ql1c               0.27409E-14   0.28033E-14  -0.33529E-13   0.36238E-12
Ql1s               0.80075E-14   0.24980E-14   0.19762E-13   0.55067E-13
Ql2c                         0.62268E+00   0.54444E+00   0.12020E+02
Ql2s                        -0.57732E-14   0.13323E-13  -0.12879E-13
Ql3c                                  -0.41300E-13   0.14122E-12
Ql3s                                   0.20872E-13  -0.47962E-13
Ql4c                                            -0.31914E+02
Ql4s                                            -0.85265E-13
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.11413E-12   0.78549E+00   0.29199E+01   0.43648E+01   0.34143E+02
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

Oxetane

Distributed multipoles for site 1 (C) at 1.95822 0.00000 0.11506

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l         0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.41725E+00   0.32500E+00  -0.54292E-01   0.34573E+00  -0.55381E+00
Ql1c              -0.58201E-01  -0.35246E+00   0.13619E+01  -0.36892E+00
Ql1s               0.30108E-14  -0.16120E-14  -0.69358E-16   0.61475E-15
Ql2c                         0.97605E-01  -0.66535E+00   0.43055E+00
Ql2s                         0.68843E-15   0.83055E-15  -0.95611E-15
Ql3c                                   0.79685E+00   0.39106E+00
Ql3s                                  -0.51800E-15   0.22168E-15
Ql4c                                             0.61955E+00
Ql4s                                            -0.37453E-15
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.41725E+00   0.33017E+00   0.36973E+00   0.17470E+01   0.10793E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

Distributed multipoles for site 2 (C) at -1.95822 0.00000 0.11506

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 l        0          1          2          3          4
- - - -
```

```
 l        0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.95457E-01  -0.19973E-01   0.46479E-01   0.67959E-01  -0.18784E+00
Ql1c                -0.10136E+00  -0.76971E-01   0.15333E+00  -0.12250E+00
Ql1s                 0.15683E+00   0.52740E-01   0.92271E-02  -0.10157E+00
Ql2c                              0.16483E-01  -0.56397E-01   0.37924E+00
Ql2s                              0.12656E-02   0.10689E+00  -0.30243E-01
Ql3c                                        -0.45856E-01  -0.17679E-01
Ql3s                                        -0.27401E-01   0.68612E-01
Ql4c                                                   -0.77075E-01
Ql4s                                                    0.72955E-01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.95457E-01   0.18779E+00   0.10554E+00   0.21371E+00   0.47078E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   7 ( C) at   0.00000  0.00000 -2.03309
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l        0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0     -0.13745E-01   0.14267E-01   0.12783E+00  -0.32774E+00  -0.87954E+00
Ql1c                -0.20142E-15   0.29078E-14  -0.39842E-15  -0.10663E-14
Ql1s                 0.15105E-14  -0.94539E-16  -0.46102E-15  -0.14498E-14
Ql2c                              0.13657E+00  -0.18726E+01   0.78463E+00
Ql2s                              0.10685E-16   0.55234E-15   0.74777E-16
Ql3c                                        -0.85785E-15  -0.89242E-15
Ql3s                                        -0.34216E-15   0.16264E-15
Ql4c                                                   -0.42799E+00
Ql4s                                                    0.12594E-15
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.13745E-01   0.14267E-01   0.18706E+00   0.19011E+01   0.12540E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   8 ( H) at   0.00000 -1.67954 -3.21574
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l        0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.12756E-01  -0.43897E-01   0.62076E-01  -0.82177E-01  -0.48413E+00
Ql1c                 0.18300E-15  -0.13083E-16   0.47584E-15  -0.10290E-14
Ql1s                -0.15429E+00  -0.15756E-01   0.21323E-01  -0.57918E-01
Ql2c                              0.91349E-01   0.25996E+00   0.75513E+00
Ql2s                              0.20286E-15   0.12847E-15   0.16691E-15
Ql3c                                        -0.55298E-16  -0.12986E-15
Ql3s                                        -0.21005E-01  -0.28912E-01
Ql4c                                                    0.21578E+00
Ql4s                                                   -0.16698E-15
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.12756E-01   0.16041E+00   0.11156E+00   0.27428E+00   0.92485E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site   9 ( H) at   0.00000  1.67954 -3.21574
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 l        0          1          2          3          4
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
Ql0      0.12756E-01  -0.43897E-01   0.62076E-01  -0.82177E-01  -0.48413E+00
Ql1c                 0.17977E-15  -0.62921E-17   0.48037E-15  -0.99336E-15
Ql1s                 0.15429E+00   0.15756E-01  -0.21323E-01   0.57918E-01
Ql2c                              0.91349E-01   0.25996E+00   0.75513E+00
Ql2s                             -0.21552E-15  -0.12652E-15  -0.13902E-15
Ql3c                                        -0.75188E-16  -0.12901E-15
Ql3s                                         0.21005E-01   0.28912E-01
Ql4c                                                    0.21578E+00
Ql4s                                                    0.17192E-15
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
|Q|      0.12756E-01   0.16041E+00   0.11156E+00   0.27428E+00   0.92485E+00
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

Distributed multipoles for site  10 ( O) at   0.00000  0.00000  2.01689
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 l        0          1          2          3          4
- - - -
```

Distributed multipoles for site 3 (C) at -2.21433 0.00000 0.66233

l	0	1	2	3	4
Ql0	0.52141E+00	0.17271E+00	-0.96137E-01	0.11283E+01	-0.40599E+00
Ql1c		0.21623E+00	0.37743E+00	-0.85120E+00	0.35535E+00
Ql1s		0.19452E-14	0.41248E-16	0.10604E-15	-0.44597E-15
Ql2c			0.17526E+00	-0.40805E+00	-0.61692E+00
Ql2s			-0.37234E-15	0.24298E-15	0.81454E-15
Ql3c				-0.99977E+00	-0.12068E+01
Ql3s				-0.61349E-16	0.15189E-14
Ql4c					0.16186E+01
Ql4s					-0.33157E-15
|Q|	0.52141E+00	0.27674E+00	0.42710E+00	0.17787E+01	0.21789E+01

Distributed multipoles for site 4 (C) at 1.25762 0.00000 -2.00613

l	0	1	2	3	4
Ql0	-0.60334E-01	0.72531E-02	0.78359E-01	-0.57955E+00	-0.12251E+01
Ql1c		0.15609E+00	0.11748E+00	-0.19784E+01	0.61371E+00
Ql1s		0.25325E-14	-0.12846E-15	-0.11034E-15	-0.23466E-15
Ql2c			-0.80668E-01	0.37867E+00	0.80153E-01
Ql2s			-0.45271E-15	0.27775E-15	0.13869E-14
Ql3c				-0.11780E+01	0.78697E+00
Ql3s				0.99680E-15	-0.49562E-15
Ql4c					0.26648E+01
Ql4s					-0.14847E-14
|Q|	0.60334E-01	0.15626E+00	0.16263E+00	0.24044E+01	0.30991E+01

Distributed multipoles for site 5 (C) at -1.25762 0.00000 -2.00613

l	0	1	2	3	4
Ql0	-0.60334E-01	0.72531E-02	0.78359E-01	-0.57955E+00	-0.12251E+01
Ql1c		-0.15609E+00	-0.11748E+00	0.19784E+01	-0.61371E+00
Ql1s		0.25045E-14	-0.12330E-15	-0.45428E-15	-0.26268E-15
Ql2c			-0.80668E-01	0.37867E+00	0.80153E-01
Ql2s			0.57642E-15	-0.31817E-15	-0.16902E-14
Ql3c				0.11780E+01	-0.78697E+00
Ql3s				0.95805E-15	-0.31404E-15
Ql4c					0.26648E+01
Ql4s					0.98551E-15
|Q|	0.60334E-01	0.15626E+00	0.16263E+00	0.24044E+01	0.30991E+01

Distributed multipoles for site 6 (H) at 2.47714 0.00000 -3.64344

l	0	1	2	3	4
Ql0	0.81439E-02	-0.18163E+00	-0.88552E-02	0.31381E-01	-0.20790E-01
Ql1c		0.13339E+00	0.39263E-01	-0.70059E-01	-0.14657E+00
Ql1s		0.15528E-15	0.14899E-15	0.12521E-15	0.87828E-16
Ql2c			0.22274E-02	0.50616E-01	0.13784E+00
Ql2s			-0.11117E-15	-0.16940E-15	-0.20415E-15
Ql3c				-0.38139E-01	-0.91659E-01
Ql3s				0.73975E-16	0.14992E-15
Ql4c					0.51069E-01
Ql4s					-0.49797E-16
|Q|	0.81439E-02	0.22535E+00	0.40310E-01	0.99547E-01	0.22787E+00

Distributed multipoles for site 7 (H) at -2.47714 0.00000 -3.64344

l	0	1	2	3	4
Ql0	0.81439E-02	-0.18163E+00	-0.88552E-02	0.31381E-01	-0.20790E-01
Ql1c		-0.13339E+00	-0.39263E-01	0.70059E-01	0.14657E+00
Ql1s		0.17192E-15	0.15993E-15	0.12400E-15	0.75789E-16
Ql2c			0.22274E-02	0.50616E-01	0.13784E+00
Ql2s			0.11800E-15	0.17116E-15	0.18974E-15
Ql3c				0.38139E-01	0.91659E-01
Ql3s				0.70944E-16	0.13804E-15
Ql4c					0.51069E-01
Ql4s					0.37968E-16
|Q|	0.81439E-02	0.22535E+00	0.40310E-01	0.99547E-01	0.22787E+00

Distributed multipoles for site 8 (H) at 3.35248 1.67452 1.09067

l	0	1	2	3	4
Ql0	-0.97361E-01	0.60432E-01	0.11648E-01	-0.34691E-02	0.38677E-01
Ql1c		0.11560E+00	-0.21950E-01	0.13356E-01	0.62087E-02
Ql1s		0.17314E+00	-0.23558E-01	0.22671E-01	-0.59853E-01
Ql2c			0.14718E-01	0.27824E-01	0.15854E-01
Ql2s			-0.48236E-01	0.21320E-01	-0.19122E-01
Ql3c				-0.18371E-01	-0.56319E-01
Ql3s				0.22948E-01	-0.72818E-01
Ql4c					0.71085E-01
Ql4s					-0.29109E-01
|Q|	0.97361E-01	0.21678E+00	0.60958E-01	0.52889E-01	0.14180E+00

Distributed multipoles for site 9 (H) at 3.35248 -1.67452 1.09067

l	0	1	2	3	4
Ql0	-0.97361E-01	0.60432E-01	0.11648E-01	-0.34691E-02	0.38677E-01
Ql1c		0.11560E+00	-0.21950E-01	0.13356E-01	0.62087E-02
Ql1s		-0.17314E+00	0.23558E-01	-0.22671E-01	0.59853E-01
Ql2c			0.14718E-01	0.27824E-01	0.15854E-01
Ql2s			0.48236E-01	-0.21320E-01	0.19122E-01
Ql3c				-0.18371E-01	-0.56319E-01
Ql3s				-0.22948E-01	0.72818E-01
Ql4c					0.71085E-01
Ql4s					0.29109E-01
|Q|	0.97361E-01	0.21678E+00	0.60958E-01	0.52889E-01	0.14180E+00

Distributed multipoles for site 10 (H) at -3.35248 -1.67452 1.09067

l	0	1	2	3	4
Ql0	-0.97361E-01	0.60432E-01	0.11648E-01	-0.34691E-02	0.38677E-01
Ql1c		-0.11560E+00	0.21950E-01	-0.13356E-01	-0.62087E-02
Ql1s		-0.17314E+00	0.23558E-01	-0.22671E-01	0.59853E-01
Ql2c			0.14718E-01	0.27824E-01	0.15854E-01
Ql2s			-0.48236E-01	0.21320E-01	-0.19122E-01
Ql3c				0.18371E-01	0.56319E-01
Ql3s				-0.22948E-01	0.72818E-01
Ql4c					0.71085E-01
Ql4s					-0.29109E-01
|Q|	0.97361E-01	0.21678E+00	0.60958E-01	0.52889E-01	0.14180E+00

Distributed multipoles for site 11 (H) at -3.35248 1.67452 1.09067

l	0	1	2	3	4
Ql0	-0.97361E-01	0.60432E-01	0.11648E-01	-0.34691E-02	0.38677E-01
Ql1c		-0.11560E+00	0.21950E-01	-0.13356E-01	-0.62087E-02
Ql1s		0.17314E+00	-0.23558E-01	0.22671E-01	-0.59853E-01
Ql2c			0.14718E-01	0.27824E-01	0.15854E-01
Ql2s			0.48236E-01	-0.21320E-01	0.19122E-01
Ql3c				0.18371E-01	0.56319E-01
Ql3s				0.22948E-01	-0.72818E-01
Ql4c					0.71085E-01
Ql4s					0.29109E-01
|Q|	0.97361E-01	0.21678E+00	0.60958E-01	0.52889E-01	0.14180E+00

Total multipoles at the origin

l	0	1	2	3	4
Ql0	-0.37859E-13	-0.66135E+00	-0.26898E+01	-0.16609E+02	-0.21342E+02
Ql1c		-0.60812E-13	0.45242E-14	-0.78160E-13	0.14895E-11
Ql1s		0.13593E-13	0.36082E-15	0.88374E-13	-0.41744E-13
Ql2c			0.32243E+01	-0.87896E+01	0.94746E+02
Ql2s			0.29532E-13	0.77272E-13	-0.12612E-12
Ql3c				-0.14344E-12	-0.19718E-12
Ql3s				0.76827E-13	-0.15987E-13
Ql4c					-0.26202E+02
Ql4s					0.39702E-12
|Q|	0.37859E-13	0.66135E+00	0.41989E+01	0.18792E+02	0.10059E+03