Supplemental Coordinates

ts for alpha glucose with water bridging O5 and O1

```
E(RBPW91) =  -763.307605474 Hartrees
Atomic numbers                             I   N=          27
           6           6           6           6           6           6
           8           8           8           8           8           8
           1           1           1           1           1           1
           1           1           1           1           1           1
           8           1           1
Current cartesian coordinates              R   N=          81
  2.35815333E+00  2.31277176E+00  7.27185518E-01  3.40890869E+00 -3.57700236E-01
  9.92248247E-01  1.81572442E+00 -2.26495681E+00 -4.65612875E-01 -8.84542824E-01
 -2.31829047E+00  4.95327526E-01 -2.13044250E+00  2.47753368E-01  1.04428302E-01
 -4.89010552E+00  3.01271601E-01  9.77606898E-01  2.51878452E+00  3.24012483E+00
 -1.53848421E+00  5.92143359E+00 -3.91304607E-01  6.31305615E-02  2.80384176E+00
 -4.73342158E+00 -1.86278689E-01 -2.32494492E+00 -4.15773178E+00 -8.14361306E-01
 -7.23230137E-01  2.07628331E+00  1.54504880E+00 -6.47946159E+00 -9.92454334E-01
 -7.09484438E-01  2.83848495E+00  3.55859316E+00  2.32762575E+00  3.48780666E+00
 -9.17371852E-01  2.98382926E+00  1.79235690E+00 -1.70087064E+00 -2.47010928E+00
 -8.60873556E-01 -2.73477674E+00  2.53811615E+00 -2.06691292E+00  7.34108146E-01
 -1.91427011E+00 -5.54138133E+00  2.26692990E+00  1.04537159E+00 -5.00023118E+00
 -4.41254801E-01  2.92128776E+00  5.88081379E+00  6.78733514E-01 -1.42689829E+00
  4.59718147E+00 -4.59507097E+00 -5.12986643E-01 -1.29568124E+00 -5.66654663E+00
 -8.76959192E-01 -5.75578823E+00 -2.66208327E+00 -9.19810174E-01 -1.21233813E+00
  4.07968043E+00  6.86372128E-01 -9.14409655E-01  6.02680410E+00 -6.14265295E-01
  8.12558840E-01  5.13208624E+00 -1.39669335E+00 -2.15827819E+00  6.19634871E+00
 -1.93442068E+00
```

ts for beta glucose with water bridging O5 and O1

```
E(RBPW91) =  -763.304396431 Hartrees
Atomic numbers                             I   N=          27
           6           6           6           6           6           6
           8           8           8           8           8           8
           1           1           1           1           1           1
           1           1           1           1           1           1
           8           1           1
Current cartesian coordinates              R   N=          81
  2.94075873E+00  9.91036359E-01 -6.02512239E-01  2.85356859E+00 -1.68045480E+00
  4.48711619E-01  4.66380202E-01 -3.04008641E+00 -3.89442027E-01 -1.91358050E+00
 -1.70370652E+00  5.26709746E-01 -2.00658155E+00  1.05046860E+00 -3.48292199E-01
 -4.35393502E+00  2.44130302E+00  6.15668966E-01  4.76550715E+00  2.41826375E+00
  1.27302792E-01  4.91927640E+00 -3.09811517E+00 -4.97405803E-01  3.45335916E-01
 -5.53045384E+00  5.83651449E-01 -4.09160203E+00 -2.96933409E+00 -3.82150376E-01
  2.19734904E-01  2.19503170E+00  6.54362466E-01 -6.55957916E+00  1.63841652E+00
 -6.22332686E-01  2.37489005E+00  1.07698730E+00 -2.62020272E+00  2.91202913E+00
 -1.54935132E+00  2.52278830E+00  4.36219416E-01 -3.08028155E+00 -2.47384456E+00
 -1.88755965E+00 -1.70286836E+00  2.61034076E+00 -2.01059601E+00  1.12930544E+00
 -2.42717244E+00 -4.13980522E+00  4.46490585E+00  2.27939834E-01 -4.46431025E+00
  2.21395534E+00  2.68563964E+00  6.42777144E+00 -2.15592982E+00 -8.33529314E-02
  1.93221589E+00 -6.32896604E+00  1.62454558E-01 -3.83927442E+00 -4.74374309E+00
 -2.42813704E-02 -6.58579712E+00 -1.89706708E-01 -5.05794988E-01  7.23969710E-01
  4.32028846E+00  2.49586855E-01  2.16632136E+00  6.12367456E+00 -2.23003428E-01
  3.74601730E+00  4.76479624E+00 -1.84168152E-01  2.33461058E+00  7.20937936E+00
  1.23160872E+00
```

ts for alpha glucose with water bonding OH1

```
E(RBPW91) =  -763.229409124 Hartrees
Atomic numbers                                 I   N=          27
           6           6           6           6           6           6
           8           8           8           8           8           8
           8           1           1           1           1           1
           1           1           1           1           1           1
           1           1           1
Current cartesian coordinates                  R   N=          81
  1.99696188E+00 -8.05668257E-01 -1.39744806E+00  1.19546343E+00  1.97203569E+00
 -1.75704580E+00 -4.30956052E-01  2.73093022E+00  4.77442903E-01 -2.72323479E+00
  1.01039863E+00  7.07659909E-01 -1.92174509E+00 -1.77388019E+00  7.01062163E-01
 -4.15942462E+00 -3.56346371E+00  4.22531998E-01  3.31827773E+00 -1.14506425E+00
  7.31921244E-01  3.37850185E+00  3.51259517E+00 -1.93934049E+00 -1.15496758E+00
  5.29905519E+00  1.70051657E-01 -4.16229618E+00  1.67619516E+00  2.89205806E+00
 -3.44461515E-01 -2.26914163E+00 -1.41331675E+00 -5.28260726E+00 -3.32809012E+00
 -1.98660203E+00  8.09459535E+00 -2.76188987E+00  1.73169430E+00  2.92620967E+00
 -1.46673116E+00 -3.15643743E+00  5.52466524E-02  2.11360630E+00 -3.49588062E+00
  7.47406912E-01  2.50314335E+00  2.18270893E+00 -3.98859710E+00  1.33158466E+00
 -8.98716481E-01 -8.92424127E-01 -2.18678683E+00  2.46557795E+00 -3.50385814E+00
 -5.51120715E+00  7.63744523E-01 -5.59889861E+00 -3.10473164E+00  1.83556184E+00
  2.77029632E+00  5.22493715E+00 -1.76252996E+00 -2.47099898E+00  5.59040280E+00
  1.40247828E+00 -3.12282961E+00  1.28461406E+00  4.34219191E+00 -3.86352221E+00
 -3.28587513E+00 -3.14100158E+00  6.30085196E+00 -3.55467362E+00  1.49177948E+00
  9.03992471E+00 -3.13719052E+00  1.93940111E-01  7.08246479E+00 -1.09248391E+00
  1.35963627E+00
```

ts for beta glucose with water bonding OH1

```
E(RBPW91) =  -763.221200048 Hartrees
Atomic numbers                                 I   N=          27
           6           6           6           6           6           6
           8           8           8           8           8           8
           8           1           1           1           1           1
           1           1           1           1           1           1
           1           1           1
Current cartesian coordinates                  R   N=          81
 -2.15369308E+00  2.70861805E-02 -6.38925360E-01 -9.39216557E-01  2.32213495E+00
  6.75263717E-01  1.72750005E+00  2.72886050E+00 -3.00818396E-01  3.34597837E+00
  3.83773438E-01  3.89739050E-02  2.02327276E+00 -1.90771976E+00 -1.14162483E+00
  3.32993958E+00 -4.39350503E+00 -4.83724036E-01 -4.40654449E+00 -5.13919405E-01
  2.75848873E-01 -2.43544515E+00  4.49232417E+00  2.04149101E-01  2.78712217E+00
  4.85323841E+00  9.46790198E-01  5.81679519E+00  8.10989453E-01 -9.56580266E-01
 -4.54884314E-01 -2.13887603E+00 -1.84343652E-01  3.04479685E+00 -4.93774166E+00
  2.11008419E+00 -9.39960493E+00 -1.49534598E+00 -4.21702367E-01 -2.06448650E+00
  3.63654490E-01 -2.72869010E+00 -8.69578717E-01  1.88535755E+00  2.70997220E+00
  1.58343530E+00  3.11913728E+00 -2.35493330E+00  3.62320524E+00  7.88559943E-03
  2.05427539E+00  2.00257251E+00 -1.66232944E+00 -3.22495835E+00  2.52314944E+00
 -5.90394405E+00 -1.67006346E+00  5.35404366E+00 -4.25561058E+00 -8.88377803E-01
 -1.40119680E+00  5.90554155E+00  7.21719512E-01  4.57680878E+00  4.79736189E+00
  5.81618238E-01  5.63898449E+00  9.92812894E-01 -2.76560479E+00  1.29349864E+00
 -4.52463883E+00  2.45625597E+00 -7.72173191E+00 -2.50679695E+00 -5.87326437E-01
 -9.98961888E+00 -1.79264652E+00  1.30098869E+00 -8.16965459E+00  4.50817541E-02
 -2.93714367E-01
```

ts for alpha glucose with water bridging O1 and O2

```
E(RBPW91) =  -763.279407647 Hartrees
Atomic numbers                             I   N=          27
           6          6          6           6          6          6
           8          8          8           8          8          8
           8          1          1           1          1          1
           1          1          1           1          1          1
           1          1          1
Current cartesian coordinates              R   N=          81
  1.34931771E+00 -2.41354007E+00 -8.97409741E-01  1.95046004E+00  3.16784362E-01
 -1.78157120E+00  8.20201014E-01  2.20495489E+00  4.91047034E-02 -2.01884709E+00
  1.81281018E+00  3.02249180E-01 -2.56668969E+00 -9.58223655E-01  9.41157193E-01
 -5.37164273E+00 -1.59069197E+00  7.99663677E-01  2.39506447E+00 -3.05915678E+00
  1.33785370E+00  4.64892175E+00  7.31430695E-01 -1.98025598E+00  1.44996789E+00
  4.65871406E+00 -8.17247864E-01 -3.01871277E+00  3.55843768E+00  2.08699042E+00
 -1.38372193E+00 -2.53033160E+00 -8.85972677E-01 -6.28990692E+00 -1.34070909E+00
 -1.69120380E+00  6.38361185E+00 -1.55002848E+00  1.91931853E+00  1.83686072E+00
 -3.73756450E+00 -2.43536785E+00  1.12702632E+00  6.10170469E-01 -3.66051554E+00
  1.66317512E+00  1.87984023E+00  1.93460464E+00 -2.94765526E+00  2.26042294E+00
 -1.49214999E+00 -1.82879998E+00 -1.39813458E+00  2.84011706E+00 -5.65245000E+00
 -3.51869239E+00  1.52871003E+00 -6.44366479E+00 -2.81002349E-01  1.98801877E+00
  4.84094299E+00  2.53802999E+00 -2.21746986E+00  3.90814865E-01  5.81721447E+00
  1.18683014E-01 -2.47314566E+00  3.02022116E+00  3.74500889E+00 -5.12725732E+00
 -2.30664550E+00 -2.71895579E+00  5.41822454E+00 -3.13364244E+00  1.21634866E+00
  6.20776542E+00 -4.40337024E-01  3.57883953E-01  4.52957271E+00 -1.28929496E+00
  2.56006262E+00
```

ts for beta glucose with water bridging O1 and O2

```
E(RBPW91) =  -763.277702442 Hartrees
Atomic numbers                             I   N=          27
           6          6          6           6          6          6
           8          8          8           8          8          8
           8          1          1           1          1          1
           1          1          1           1          1          1
           1          1          1
Current cartesian coordinates              R   N=          81
 -1.78700355E+00 -1.50447692E+00 -1.12177755E+00 -1.99336269E+00  9.94440947E-01
  3.75109669E-01  1.41603895E-01  2.75679871E+00 -3.33313146E-01  2.68372927E+00
  1.50514403E+00  1.55457922E-01  2.76938957E+00 -1.09223829E+00 -1.13205474E+00
  5.06637640E+00 -2.63705602E+00 -3.28697044E-01 -3.60601696E+00 -3.20067564E+00
 -6.05361655E-01 -4.37059797E+00  2.21607944E+00 -1.22161902E-01 -1.68040006E-01
  5.02618738E+00  1.05175729E+00  4.67477041E+00  3.14415708E+00 -6.00728114E-01
  6.40194264E-01 -2.54973910E+00 -4.22218503E-01  4.93047478E+00 -3.27023608E+00
  2.25440867E+00 -7.33137384E+00 -1.60843984E+00  7.07187459E-01 -1.68580216E+00
 -1.03991761E+00 -3.17134766E+00 -1.85626336E+00  5.20111768E-01  2.39573445E+00
 -1.24910772E-02  3.14903614E+00 -2.38342733E+00  2.93797303E+00  1.22271954E+00
  2.18921771E+00  2.80899283E+00 -8.13485615E-01 -3.20829830E+00  5.17870543E+00
 -4.33182143E+00 -1.53002312E+00  6.78625749E+00 -1.52303894E+00 -6.06453837E-01
 -4.19393274E+00  3.92827517E+00  5.00436811E-01  1.39222582E+00  5.95914055E+00
  8.67419833E-01  4.65240106E+00  3.23703397E+00 -2.42493726E+00  3.27703237E+00
 -4.02000041E+00  2.47259165E+00 -6.32364569E+00 -2.24672700E+00 -9.21336558E-01
 -6.78308727E+00  1.99311129E-01  6.55111744E-01 -5.61804854E+00 -2.43497793E+00
  1.37389523E+00
```

Gaussian job files

To generate alpha ts with water bridging OH1 and O5

```
%Chk=alpha1w

# b3pw91/6-31G** opt=(qst2) test

substrate here

   0   1
 C
 C,1,R2
 C,2,R3,1,A3
 C,3,R4,2,A4,1,D4,0
 C,4,R5,3,A5,2,D5,0
 C,5,R6,4,A6,3,D6,0
 O,1,R7,2,A7,3,D7,0
 O,2,R8,1,A8,3,D8,0
 O,3,R9,2,A9,4,D9,0
 O,4,R10,3,A10,5,D10,0
 O,1,R11,2,A11,7,D11,0
 O,6,R12,5,A12,4,D12,0
 H,1,R13,2,A13,7,D13,0
 H,2,R14,1,A14,3,D14,0
 H,3,R15,2,A15,4,D15,0
 H,4,R16,3,A16,5,D16,0
 H,5,R17,4,A17,6,D17,0
 H,6,R18,5,A18,12,D18,0
 H,6,R19,5,A19,12,D19,0
 H,8,R20,2,A20,1,D20,0
 H,9,R21,3,A21,2,D21,0
 H,10,R22,4,A22,3,D22,0
 H,12,R23,6,A23,5,D23,0
 H,11,R26,5,A26,17,D26,0
 O,17,R25,5,A25,4,D25,0
 H,7,R24,1,A24,2,D24,0
 H,25,R27,17,A27,24,D27,0
      Variables:
 R2=1.5393687
 R3=1.52964636
 R4=1.52924851
 R5=1.53738154
 R6=1.53494918
 R7=1.42178937
 R8=1.43726685
 R9=1.4368121
 R10=1.43341341
 R11=1.42403406
 R12=1.42372013
 R13=1.09486529
 R14=1.09583986
 R15=1.09697128
 R16=1.09763245
 R17=1.09841522
 R18=1.09553503
 R19=1.09463693
 R20=0.97971118
 R21=0.97852542
```

R22=0.981265
R23=0.981697
R24=0.98685815
R25=4.02881893
R26=3.2837
R27=0.97209722
A3=110.19937448
A4=110.19755194
A5=109.54685939
A6=110.96586677
A7=108.71641185
A8=111.32781477
A9=110.33741301
A10=109.72054365
A11=112.08047248
A12=112.37270549
A13=109.03894258
A14=110.20578784
A15=111.20578226
A16=109.08235441
A17=109.45062172
A18=110.11208562
A19=110.89560202
A20=105.23397672
A21=105.22429377
A22=104.63673953
A23=106.77337984
A24=104.34132674
A25=98.12031702
A26=116.5669
A27=148.45505954
D4=-52.69856293
D5=54.85661949
D6=-178.35150386
D7=-69.08655886
D8=120.28133947
D9=-120.13260855
D10=122.63327311
D11=122.74345189
D12=-66.65819506
D13=-116.92265772
D14=-120.6415399
D15=123.0014281
D16=-120.61625431
D17=-118.13542231
D18=-120.4175356
D19=121.93195121
D20=-38.29844489
D21=-45.40669081
D22=44.27453449
D23=41.68445672
D24=-164.1356796
D25=-135.33982452
D26=36.6177
D27=-94.65338531

product here

```
   0   1
C    1.896  -1.455   0.177
C    1.435  -0.591   1.341
C   -0.088  -0.430   1.473
C   -0.716   0.776   0.737
C   -0.587   0.737  -0.796
C   -1.483   1.776  -1.489
O    1.153  -2.105  -0.556
O    1.921  -1.259   2.527
O   -0.429  -0.247   2.878
O   -2.108   0.825   1.119
O    0.772   0.982  -1.164
O   -2.866   1.475  -1.340
H    2.989  -1.476   0.024
H    1.935   0.380   1.290
H   -0.605  -1.352   1.182
H   -0.261   1.697   1.122
H   -0.884  -0.261  -1.141
H   -1.260   1.811  -2.561
H   -1.294   2.780  -1.094
H    1.484  -2.133   2.565
H    0.393  -0.405   3.388
H   -2.101   0.624   2.082
H   -2.997   1.300  -0.381
H    0.882   0.580  -2.060
O    0.996  -0.937  -3.090
H    0.983  -1.597  -2.363
H    0.835  -1.493  -3.871
```

To generate beta ts with water bridging OH1 and O5

```
%Chk=beta1w

# b3pw91/6-31G** opt=(qst2) test

substrate here

   0   1
 C
 C,1,R2
 C,2,R3,1,A3
 C,3,R4,2,A4,1,D4,0
 C,4,R5,3,A5,2,D5,0
 C,5,R6,4,A6,3,D6,0
 O,1,R7,2,A7,3,D7,0
 O,2,R8,1,A8,3,D8,0
 O,3,R9,2,A9,4,D9,0
 O,4,R10,3,A10,5,D10,0
 O,1,R11,2,A11,7,D11,0
 O,6,R12,5,A12,4,D12,0
 H,1,R13,2,A13,7,D13,0
 H,2,R14,1,A14,3,D14,0
 H,3,R15,2,A15,4,D15,0
 H,4,R16,3,A16,5,D16,0
 H,5,R17,4,A17,6,D17,0
```

```
H,6,R18,5,A18,12,D18,0
H,6,R19,5,A19,12,D19,0
H,8,R20,2,A20,1,D20,0
H,9,R21,3,A21,2,D21,0
H,10,R22,4,A22,3,D22,0
H,12,R23,6,A23,5,D23,0
H,11,R26,5,A26,17,D26,0
O,11,R25,5,A25,4,D25,0
H,7,R24,1,A24,2,D24,0
H,25,R27,26,A27,24,D27,0
     Variables:
R2=1.53693103
R3=1.52478654
R4=1.52972089
R5=1.53874852
R6=1.53451263
R7=1.42097783
R8=1.4360087
R9=1.43658414
R10=1.43208834
R11=1.42292937
R12=1.42325859
R13=1.09715769
R14=1.09723698
R15=1.09723698
R16=1.09749989
R17=1.09848851
R18=1.09509726
R19=1.09609261
R20=0.98068802
R21=0.97975558
R22=0.98126908
R23=0.98173011
R24=0.98426165
R25=3.2666
R26=2.9365
R27=0.97369656
A3=109.46575119
A4=110.19386759
A5=109.54552622
A6=111.0135213
A7=107.49560135
A8=111.45683686
A9=110.63570017
A10=109.61565274
A11=111.04960252
A12=112.05346135
A13=110.99239357
A14=110.53171024
A15=110.78243581
A16=109.17344617
A17=109.45498791
A18=110.21427477
A19=110.96649284
A20=104.69262417
A21=105.00998187
A22=104.8280151
```

```
 A23=106.83793962
 A24=104.23835842
 A25=132.6627
 A26=125.8592
 A27=146.36072708
 D4=-53.69666457
 D5=53.92195465
 D6=-178.16531924
 D7=176.25290419
 D8=120.80961622
 D9=-120.54503038
 D10=122.33642621
 D11=-119.10841239
 D12=-67.62966761
 D13=117.40132891
 D14=-121.15565412
 D15=122.63508432
 D16=-120.80370772
 D17=-118.45672702
 D18=-120.27205175
 D19=121.82704871
 D20=50.60826187
 D21=-46.52253789
 D22=46.02616155
 D23=44.0756151
 D24=170.70915389
 D25=151.5864
 D26=51.3561
 D27=146.66614584

product here

   0   1
C   -1.496   1.668  -0.009
C   -1.330   0.737   1.181
C    0.154   0.522   1.519
C    0.843  -0.686   0.847
C    0.777  -0.680  -0.691
C    1.728  -1.705  -1.326
O   -2.399   1.566  -0.840
O   -1.941   1.422   2.295
O    0.301   0.330   2.949
O    2.212  -0.697   1.298
O   -0.563  -0.974  -1.080
O    3.092  -1.352  -1.130
H   -0.794   2.519  -0.057
H   -1.865  -0.205   1.033
H    0.732   1.429   1.303
H    0.386  -1.608   1.230
H    1.045   0.320  -1.053
H    1.547  -1.771  -2.404
H    1.557  -2.706  -0.914
H   -2.900   1.441   2.109
H   -0.429   0.851   3.349
H    2.148  -0.554   2.268
H    3.187  -1.179  -0.167
H   -0.668  -0.691  -2.020
```

```
O   -1.434   0.443  -3.180
H   -2.011   0.867  -2.506
H   -1.879   0.693  -4.006
```

To generate alpha ts with water hydrogen bonded only to OH1

```
%chk=a1

#b3pw91/6-31g** opt(qst3,addredundant) iop(2/15=3) test

a1sub

  0  1
  C       -3.797   0.331   0.050
  C       -4.857   0.213   1.1450
  C       -6.113  -0.399   0.5470
  C       -6.593   0.424  -0.6420
  C       -5.460   0.642  -1.6520
  C       -5.812   1.681  -2.7080
  O       -3.460  -0.938  -0.3990
  O       -4.351  -0.554   2.2120
  O       -7.090  -0.460   1.5710
  O       -7.737  -0.186  -1.2330
  O       -4.299   1.156  -0.9930
  O       -5.998   2.957  -2.1360
  O       -1.150  -2.374  -0.4190
  H       -2.923   0.873   0.4320
  H       -5.099   1.237   1.4740
  H       -5.857  -1.414   0.1970
  H       -6.934   1.403  -0.2910
  H       -5.215  -0.316  -2.1380
  H       -5.018   1.692  -3.4710
  H       -6.751   1.400  -3.1930
  H       -5.111  -0.744   2.7780
  H       -7.926  -0.666   1.1330
  H       -7.450  -1.028  -1.6110
  H       -5.207   3.116  -1.6030
  H       -2.534  -0.994  -0.6830
  H       -0.464  -2.131   0.2130
  H       -1.852  -2.751   0.1270

1 7 13 F
2 1 7 13 F

a1ion

  0  1
  C                  -2.612   1.925  -2.000
  C                  -4.090   1.691  -2.316
  C                  -4.377   2.200  -3.719
  C                  -3.979   3.665  -3.846
  C                  -2.533   3.883  -3.384
  C                  -2.186   5.358  -3.232
  O                  -1.834   1.179  -2.874
  O                  -4.392   0.322  -2.177
  O                  -5.758   2.008  -3.970
```

```
  O                  -4.198   4.120  -5.178
  O                  -2.336   3.316  -2.086
  O                  -2.955   5.969  -2.219
  O                  -0.030  -0.829  -2.539
  H                  -2.408   1.669  -0.953
  H                  -4.674   2.300  -1.605
  H                  -3.770   1.604  -4.422
  H                  -4.637   4.275  -3.219
  H                  -1.845   3.410  -4.103
  H                  -1.108   5.448  -3.030
  H                  -2.406   5.880  -4.168
  H                  -5.273   0.211  -2.559
  H                  -5.957   2.505  -4.774
  H                  -3.581   3.643  -5.749
  H                  -2.847   5.405  -1.441
  H                   0.591  -0.172  -2.886
  H                  -0.079  -1.347  -1.727
  H                  -0.824  -1.081  -3.028

1 7 13 F
2 1 7 13 F

a1ts

  0  1
  C                  -1.187   1.892  -3.089
  C                  -2.397   1.759  -4.013
  C                  -1.973   2.111  -5.430
  C                  -1.358   3.504  -5.471
  C                  -0.242   3.643  -4.429
  C                   0.207   5.087  -4.245
  O                  -0.220   0.972  -3.467
  O                  -2.918   0.453  -3.926
  O                  -3.119   2.018  -6.257
  O                  -0.911   3.806  -6.790
  O                  -0.709   3.229  -3.142
  O                  -0.832   5.889  -3.729
  O                   0.960  -1.137  -2.218
  H                  -1.496   1.752  -2.046
  H                  -3.140   2.503  -3.684
  H                  -1.211   1.376  -5.743
  H                  -2.131   4.247  -5.249
  H                   0.616   3.021  -4.729
  H                   1.092   5.100  -3.590
  H                   0.491   5.504  -5.215
  H                  -3.551   0.377  -4.652
  H                  -2.877   2.426  -7.098
  H                  -0.181   3.204  -6.989
  H                  -1.152   5.421  -2.946
  H                   0.598   0.371  -2.305
  H                   0.492  -1.541  -1.478
  H                   0.430  -1.374  -2.990

1 7 13 F
2 1 7 13 F
7 13 F
```

To generate beta ts with water hydrogen bonded only to OH1

```
%chk=b1

#b3pw91/6-31g** opt(qst3,addredundant) iop(2/15=3) test

b1sub

  0  1
  C       -3.833   0.343  -0.3040
  C       -4.606   0.579   0.9890
  C       -5.964  -0.098   0.8870
  C       -6.726   0.348  -0.3510
  C       -5.858   0.152  -1.5980
  C       -6.466   0.786  -2.8440
  O       -2.665   1.067  -0.2700
  O       -3.865   0.056   2.0680
  O       -6.675   0.179   2.0760
  O       -7.974  -0.331  -0.4310
  O       -4.604   0.796  -1.4180
  O       -6.552   2.186  -2.7140
  O        0.037   1.214  -0.5290
  H       -3.645  -0.741  -0.4220
  H       -4.755   1.667   1.0890
  H       -5.780  -1.189   0.8010
  H       -6.975   1.411  -0.2720
  H       -5.712  -0.932  -1.7710
  H       -5.862   0.494  -3.7180
  H       -7.482   0.406  -2.9840
  H       -4.463   0.067   2.8270
  H       -7.591  -0.081   1.9100
  H       -7.788  -1.269  -0.5710
  H       -5.666   2.476  -2.4550
  H       -1.997   0.718  -0.8790
  H       -0.011   2.147  -0.7640
  H       -0.359   1.184   0.3510

1 7 13 F
2 1 7 13 F

b1ion

  0  1
  C                  3.224   2.071  -0.469
  C                  3.165   3.216  -1.474
  C                  4.525   3.364  -2.139
  C                  5.638   3.529  -1.116
  C                  5.585   2.385  -0.098
  C                  6.523   2.605   1.084
  O                  2.042   2.023   0.231
  O                  2.168   2.935  -2.430
  O                  4.454   4.461  -3.026
  O                  6.897   3.630  -1.772
  O                  4.282   2.300   0.463
  O                  6.144   3.737   1.832
  O                 -0.107   0.638   1.156
```

```
  H                  3.426   1.125  -1.006
  H                  2.939   4.136  -0.911
  H                  4.716   2.430  -2.706
  H                  5.512   4.472  -0.576
  H                  5.848   1.436  -0.604
  H                  6.532   1.693   1.700
  H                  7.537   2.782   0.713
  H                  2.288   3.586  -3.134
  H                  5.364   4.663  -3.280
  H                  7.070   2.783  -2.203
  H                  5.204   3.614   2.028
  H                  0.066  -0.236   1.078
  H                 -0.209   1.244   1.898
  H                 -0.202   1.210   0.385

1 7 13 F
2 1 7 13 F

b1ts

  0  1
  C                 -1.453   2.102  -2.894
  C                 -2.571   3.077  -2.540
  C                 -3.533   3.177  -3.714
  C                 -2.814   3.539  -5.004
  C                 -1.660   2.563  -5.251
  C                 -0.757   2.997  -6.400
  O                 -0.511   2.114  -1.893
  O                 -3.235   2.614  -1.386
  O                 -4.528   4.122  -3.377
  O                 -3.740   3.589  -6.084
  O                 -0.819   2.512  -4.106
  O                 -0.109   4.214  -6.108
  O                  1.050   0.802  -0.096
  H                 -1.884   1.094  -3.044
  H                 -2.106   4.063  -2.373
  H                 -3.992   2.175  -3.847
  H                 -2.398   4.548  -4.928
  H                 -2.074   1.559  -5.468
  H                 -0.036   2.190  -6.605
  H                 -1.363   3.155  -7.296
  H                 -4.031   3.155  -1.306
  H                 -5.002   4.319  -4.196
  H                 -4.076   2.693  -6.223
  H                  0.304   4.085  -5.242
  H                  0.236   0.726  -1.458
  H                  1.704   1.509  -0.109
  H                  0.246   1.246   0.202

1 7 13 F
2 1 7 13 F
7 13 F
```

To generate alpha ts with water bridging OH1 and OH2

```
%chk=a12
```

```
#b3pw91/6-31g** opt=qst3 iop(2/15=3) test

a12

  0  1
  C         1.715   0.237   0.753
  C         0.318   0.131   1.390
  C        -0.719   0.075   0.286
  C        -0.601   1.299  -0.610
  C         0.839   1.462  -1.110
  C         1.076   2.811  -1.776
  O         2.011  -0.846  -0.068
  O         0.233  -1.020   2.225
  O        -1.994  -0.020   0.898
  O        -1.545   1.223  -1.671
  O         1.751   1.422  -0.008
  O         0.912   3.875  -0.864
  O         2.258  -2.843   1.778
  H         2.473   0.373   1.538
  H         0.151   1.035   1.994
  H        -0.512  -0.824  -0.318
  H        -0.871   2.196  -0.042
  H         1.078   0.651  -1.816
  H         2.081   2.812  -2.224
  H         0.342   2.950  -2.575
  H        -0.709  -1.150   2.399
  H        -2.642   0.147   0.201
  H        -1.275   0.494  -2.247
  H         1.494   3.669  -0.121
  H         2.254  -1.610   0.504
  H         1.477  -2.379   2.137
  H         1.913  -3.658   1.399

a12ion

  0  1
  C                   1.564  -0.587   0.880
  C                   0.303   0.132   1.393
  C                  -0.580   0.474   0.210
  C                   0.187   1.327  -0.790
  C                   1.510   0.653  -1.169
  C                   2.437   1.582  -1.942
  O                   1.268  -1.765   0.203
  O                  -0.395  -0.685   2.328
  O                  -1.730   1.135   0.708
  O                  -0.629   1.610  -1.920
  O                   2.236   0.295   0.011
  O                   2.833   2.688  -1.160
  O                   0.382  -3.334   2.254
  H                   2.260  -0.759   1.714
  H                   0.620   1.063   1.886
  H                  -0.860  -0.474  -0.280
  H                   0.413   2.300  -0.342
  H                   1.306  -0.250  -1.765
  H                   3.305   1.003  -2.293
  H                   1.907   1.972  -2.815
```

```
  H                  -1.269  -0.285   2.427
  H                  -2.176   1.518  -0.059
  H                  -0.767   0.777  -2.393
  H                   3.200   2.312  -0.350
  H                   1.366  -3.448   2.107
  H                  -0.048  -2.489   2.492
  H                  -0.329  -3.895   1.929

a12ts

  0  1
  C                  -0.120  -0.828   1.693
  C                  -1.053   0.152   0.958
  C                  -0.385   0.589  -0.330
  C                   0.969   1.217  -0.035
  C                   1.821   0.277   0.825
  C                   3.064   0.960   1.380
  O                   0.161  -1.963   0.940
  O                  -2.313  -0.458   0.696
  O                  -1.262   1.490  -0.984
  O                   1.613   1.586  -1.248
  O                   1.081  -0.147   1.974
  O                   2.729   2.011   2.259
  O                  -2.270  -3.207   0.952
  H                  -0.546  -1.083   2.674
  H                  -1.198   1.030   1.604
  H                  -0.228  -0.313  -0.945
  H                   0.826   2.152   0.517
  H                   2.114  -0.603   0.230
  H                   3.692   0.203   1.873
  H                   3.633   1.395   0.553
  H                  -2.751   0.111   0.047
  H                  -0.747   1.907  -1.687
  H                   1.839   0.770  -1.715
  H                   2.140   1.619   2.917
  H                  -0.839  -2.786   1.579
  H                  -2.556  -2.282   0.817
  H                  -2.400  -3.636   0.100
```

To generate beta ts with water bridging OH1 and OH2

```
%chk=b12

#b3pw91/6-31g** opt=qst3 iop(2/15=3) test

b12sub

  0  1
  C         1.095  -0.093  -0.910
  C         0.471  -0.238   0.485
  C        -0.933  -0.796   0.361
  C        -1.781   0.071  -0.555
  C        -1.067   0.256  -1.899
  C        -1.739   1.304  -2.780
  O         2.314   0.548  -0.888
  O         1.268  -1.112   1.277
```

```
  O       -1.477  -0.904   1.661
  O       -3.084  -0.483  -0.688
  O        0.254   0.733  -1.694
  O       -1.674   2.582  -2.190
  O        3.881  -1.301   0.393
  H        1.163  -1.099  -1.374
  H        0.434   0.765   0.935
  H       -0.852  -1.802  -0.099
  H       -1.926   1.059  -0.105
  H       -1.046  -0.715  -2.432
  H       -1.263   1.288  -3.772
  H       -2.797   1.052  -2.899
  H        0.738  -1.340   2.052
  H       -2.425  -1.058   1.547
  H       -3.002  -1.316  -1.171
  H       -0.738   2.732  -1.999
  H        2.993  -0.097  -0.590
  H        3.058  -1.406   0.908
  H        4.459  -0.778   0.958

b12ion

  0  1
  C                  1.079  -0.085   0.929
  C                 -0.216  -0.615   0.298
  C                 -0.179  -0.398  -1.202
  C                  0.057   1.067  -1.531
  C                  1.310   1.565  -0.802
  C                  1.477   3.079  -0.891
  O                  1.054  -0.111   2.306
  O                 -0.352  -2.004   0.580
  O                 -1.389  -0.887  -1.744
  O                  0.123   1.249  -2.940
  O                  1.219   1.281   0.586
  O                  0.423   3.746  -0.235
  O                  1.084  -2.807   2.802
  H                  1.935  -0.660   0.518
  H                 -1.051  -0.048   0.735
  H                  0.676  -0.980  -1.600
  H                 -0.796   1.667  -1.196
  H                  2.200   1.070  -1.237
  H                  2.456   3.351  -0.470
  H                  1.454   3.384  -1.941
  H                 -1.048  -2.335  -0.002
  H                 -1.434  -0.555  -2.651
  H                  0.924   0.810  -3.257
  H                  0.400   3.378   0.659
  H                  2.085  -2.830   2.823
  H                  0.497  -2.796   2.022
  H                  0.493  -2.922   3.553

b12ts

  0  1
  C                  1.089   0.013   0.922
  C                 -0.206  -0.587   0.357
  C                 -0.186  -0.511  -1.157
```

C	0.031	0.919	-1.625
C	1.285	1.496	-0.959
C	1.434	2.996	-1.191
O	1.078	0.116	2.295
O	-0.324	-1.944	0.769
O	-1.396	-1.060	-1.639
O	0.081	0.969	-3.045
O	1.211	1.343	0.450
O	0.379	3.711	-0.589
O	1.142	-2.522	3.041
H	1.947	-0.589	0.557
H	-1.043	0.010	0.748
H	0.672	-1.119	-1.510
H	-0.825	1.539	-1.338
H	2.177	0.972	-1.355
H	2.415	3.317	-0.807
H	1.398	3.202	-2.265
H	-1.023	-2.335	0.228
H	-1.453	-0.815	-2.572
H	0.883	0.511	-3.328
H	0.369	3.429	0.336
H	1.594	-1.256	2.670
H	0.547	-2.589	2.270
H	0.560	-2.571	3.806

Full Reference

(23) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 94, Revisions C.2, D.4, Gaussian 98, Revision A.6*; Gaussian, Inc.: Pittsburgh, PA, 1998.