Cartesian Coordinates:

H2O:

H	1	0.00000000	-1.43311281	0.99231287
O	8	0.00000000	-0.00000000	-0.12504946
H	1	0.00000000	1.43311281	0.99231287

HOF:

F	9	-1.29514358	0.01089617	0.00000000
O	8	1.42747766	-0.11906730	0.00000000
H	1	1.75950841	1.68428192	0.00000000

HOCl:

CL	17	-1.06107266	0.00693987	0.00000000
O	8	2.15440561	-0.11896856	0.00000000
H	1	2.62442350	1.64732245	0.00000000

HOBr:

BR	35	-0.61943585	0.00283401	0.00000000
O	8	2.84745363	-0.11785894	-0.00000000
H	1	3.31413581	1.64858843	0.00000000

FOH-OH2-syn:

F	9	-2.33964937	1.07579065	0.00000000
O	8	-1.36005677	-1.47839810	0.00000000
H	1	0.44100442	-1.03018546	0.00000000
O	8	3.61532258	0.11671255	0.00000000
H	1	3.93538686	1.18075373	-1.44093076
H	1	3.93538686	1.18075373	1.44093076

FOH-OH2-anti:

F	9	-2.59718447	0.95867694	-0.00000000
O	8	-1.25015977	-1.41716591	0.00000000
H	1	0.47063439	-0.73317909	0.00000000
O	8	3.70432042	0.32017526	-0.00000000
H	1	4.76965250	0.03564946	1.44518853
H	1	4.76965250	0.03564946	-1.44518853

ClOH-OH2-syn:

CL	17	-2.16478337	0.65875083	0.00000000
O	8	-0.30396261	-1.95676968	0.00000000
H	1	1.39308672	-1.21905624	0.00000000
O	8	4.37507892	0.40423151	0.00000000
H	1	4.55378909	1.50102944	-1.44088559
H	1	4.55378909	1.50102944	1.44088559

ClOH-OH2-anti:

CL	17	-2.32804044	0.58347211	0.00000000
O	8	-0.19192972	-1.81205507	0.00000000
H	1	1.42362619	-0.91587960	0.00000000
O	8	4.49169962	0.56098119	0.00000000
H	1	5.55636356	0.26319848	1.44382268
H	1	5.55636356	0.26319848	-1.44382268

BrOH-OH2-anti:

BR	35	-1.51761724	0.27686036	0.00000000
O	8	1.01279408	-2.08027971	0.00000000
H	1	2.53804023	-1.04033843	0.00000000
O	8	5.48718947	0.71759022	0.00000000
H	1	6.57021047	0.49374751	1.44295826
H	1	6.57021047	0.49374751	-1.44295826

HOCl-OH2-anti:

```
H         1        -4.32283200     1.57988307     0.00000000
O         8        -3.80456733    -0.17155133     0.00000000
CL       17        -0.58324797     0.04354472    -0.00000000
O         8         4.69613090     0.09056273    -0.00000000
H         1         5.20511357    -0.90271069     1.43595483
H         1         5.20511357    -0.90271069    -1.43595483


HOBr-OH2-syn:
H         1        -4.13856034     1.85325422     0.00000000
O         8        -3.79387545     0.06120917     0.00000000
BR       35        -0.31240787    -0.05895827     0.00000000
O         8         4.90157795    -0.00383130     0.00000000
H         1         5.51090038     0.92643971     1.43868830
H         1         5.51090038     0.92643971    -1.43868830

HOBr-OH2-anti:
H         1        -4.29717123     1.57250529    -0.00000000
O         8        -3.78531433    -0.17950082    -0.00000000
BR       35        -0.30796372     0.02267722    -0.00000000
O         8         4.88362889     0.07650573    -0.00000000
H         1         5.49070170    -0.85682599    -1.43809974
H         1         5.49070170    -0.85682599     1.43809974




SAPT Results:

FOH-OH2-syn:
    SAPT Results
  ------------------------------------------------------------------------------
    Electrostatics               -20.44352806 [mEh]     -12.82850754 [kcal/mol]
      Elst10,r                   -21.62116698 [mEh]     -13.56748712 [kcal/mol]
      Elst12,r                     0.92867813 [mEh]       0.58275432 [kcal/mol]
      Elst13,r                     0.24896079 [mEh]       0.15622526 [kcal/mol]

    Exchange                      21.03789192 [mEh]      13.20147649 [kcal/mol]
      Exch10                      18.31105932 [mEh]      11.49036320 [kcal/mol]
      Exch10(S^2)                 18.11619644 [mEh]      11.36808489 [kcal/mol]
      Exch11(S^2)                  0.17617818 [mEh]       0.11055348 [kcal/mol]
      Exch12(S^2)                  2.55065442 [mEh]       1.60055981 [kcal/mol]

    Induction                     -8.52285028 [mEh]      -5.34816930 [kcal/mol]
      Ind20,r                    -10.00103470 [mEh]      -6.27574402 [kcal/mol]
      Ind30,r                    -12.16889253 [mEh]      -7.63609535 [kcal/mol]
      Ind22                       -1.20802493 [mEh]      -0.75804709 [kcal/mol]
      Exch-Ind20,r                 5.30047213 [mEh]       3.32609647 [kcal/mol]
      Exch-Ind30,r                10.85275999 [mEh]       6.81020971 [kcal/mol]
      Exch-Ind22                   0.64024400 [mEh]       0.40175918 [kcal/mol]
      delta HF,r (2)              -3.25450678 [mEh]      -2.04223384 [kcal/mol]
      delta HF,r (3)              -1.93837424 [mEh]      -1.21634820 [kcal/mol]

    Dispersion                    -5.94711738 [mEh]      -3.73187250 [kcal/mol]
      Disp20                      -5.84868162 [mEh]      -3.67010312 [kcal/mol]
      Disp30                       0.20994550 [mEh]       0.13174279 [kcal/mol]
      Disp21                       0.15949619 [mEh]       0.10008537 [kcal/mol]
      Disp22 (SDQ)                -0.11889980 [mEh]      -0.07461075 [kcal/mol]
      Disp22 (T)                  -0.84269317 [mEh]      -0.52879795 [kcal/mol]
      Est. Disp22 (T)             -0.99216023 [mEh]      -0.62258994 [kcal/mol]
      Exch-Disp20                  1.08482856 [mEh]       0.68074020 [kcal/mol]
      Exch-Disp30                 -0.07201762 [mEh]      -0.04519174 [kcal/mol]
      Ind-Disp30                  -1.91280583 [mEh]      -1.20030378 [kcal/mol]
      Exch-Ind-Disp30              1.54317746 [mEh]       0.96835848 [kcal/mol]

  Total HF                        -11.26517702 [mEh]      -7.06900530 [kcal/mol]
  Total SAPT0                     -16.02903008 [mEh]     -10.05836823 [kcal/mol]
  Total SAPT2                     -12.94130028 [mEh]      -8.12078853 [kcal/mol]
  Total SAPT2+                    -13.89286411 [mEh]      -8.71790385 [kcal/mol]
  Total SAPT2+(3)                 -13.43395782 [mEh]      -8.42993580 [kcal/mol]
```

```
  Total SAPT2+3                  -13.87560381 [mEh]      -8.70707284 [kcal/mol]

  Special recipe for scaled SAPT0 (see Manual):
    Electrostatics sSAPT0         -21.62116698 [mEh]     -13.56748712 [kcal/mol]
    Exchange sSAPT0                18.31105932 [mEh]      11.49036320 [kcal/mol]
    Induction sSAPT0               -7.78218291 [mEh]      -4.88339350 [kcal/mol]
    Dispersion sSAPT0              -4.72846901 [mEh]      -2.96715910 [kcal/mol]
  Total sSAPT0                   -15.82075959 [mEh]      -9.92767652 [kcal/mol]
  ---------------------------------------------------------------------------



FOH-OH2-anti:

  SAPT Results
---------------------------------------------------------------------------
  Electrostatics               -18.41938439 [mEh]     -11.55833869 [kcal/mol]
    Elst10,r                   -19.61867937 [mEh]     -12.31090768 [kcal/mol]
    Elst12,r                     1.08804619 [mEh]       0.68275932 [kcal/mol]
    Elst13,r                     0.11124879 [mEh]       0.06980967 [kcal/mol]

  Exchange                      18.34295392 [mEh]      11.51037784 [kcal/mol]
    Exch10                      16.11719742 [mEh]      10.11369449 [kcal/mol]
    Exch10(S^2)                 15.96107046 [mEh]      10.01572335 [kcal/mol]
    Exch11(S^2)                  0.18178620 [mEh]       0.11407257 [kcal/mol]
    Exch12(S^2)                  2.04397030 [mEh]       1.28261078 [kcal/mol]

  Induction                     -7.47648195 [mEh]      -4.69156345 [kcal/mol]
    Ind20,r                     -8.52265559 [mEh]      -5.34804735 [kcal/mol]
    Ind30,r                     -9.75846596 [mEh]      -6.12353010 [kcal/mol]
    Ind22                       -0.89276179 [mEh]      -0.56021651 [kcal/mol]
    Exch-Ind20,r                 4.28710152 [mEh]       2.69019693 [kcal/mol]
    Exch-Ind30,r                 8.64573231 [mEh]       5.42527916 [kcal/mol]
    Exch-Ind22                   0.44908073 [mEh]       0.28180243 [kcal/mol]
    delta HF,r (2)              -2.79724682 [mEh]      -1.75529895 [kcal/mol]
    delta HF,r (3)              -1.68451317 [mEh]      -1.05704801 [kcal/mol]

  Dispersion                    -5.32013302 [mEh]      -3.33843401 [kcal/mol]
    Disp20                      -5.25641799 [mEh]      -3.29845223 [kcal/mol]
    Disp30                       0.18788005 [mEh]       0.11789652 [kcal/mol]
    Disp21                       0.16854474 [mEh]       0.10576343 [kcal/mol]
    Disp22 (SDQ)                -0.08336141 [mEh]      -0.05231007 [kcal/mol]
    Disp22 (T)                  -0.75012960 [mEh]      -0.47071345 [kcal/mol]
    Est. Disp22 (T)             -0.88117524 [mEh]      -0.55294583 [kcal/mol]
    Exch-Disp20                  0.93088096 [mEh]       0.58413665 [kcal/mol]
    Exch-Disp30                 -0.06514400 [mEh]      -0.04087848 [kcal/mol]
    Ind-Disp30                  -1.57345041 [mEh]      -0.98735508 [kcal/mol]
    Exch-Ind-Disp30              1.25211026 [mEh]       0.78571109 [kcal/mol]

Total HF                        -10.53428284 [mEh]      -6.61036256 [kcal/mol]
Total SAPT0                     -14.85981987 [mEh]      -9.32467814 [kcal/mol]
Total SAPT2                     -11.98969823 [mEh]      -7.52364954 [kcal/mol]
Total SAPT2+                    -12.78569014 [mEh]      -8.02314203 [kcal/mol]
Total SAPT2+(3)                 -12.48656130 [mEh]      -7.83543584 [kcal/mol]
Total SAPT2+3                   -12.87304544 [mEh]      -8.07795831 [kcal/mol]

Special recipe for scaled SAPT0 (see Manual):
  Electrostatics sSAPT0         -19.61867937 [mEh]     -12.31090768 [kcal/mol]
  Exchange sSAPT0                16.11719742 [mEh]      10.11369449 [kcal/mol]
  Induction sSAPT0               -6.90576041 [mEh]      -4.33343026 [kcal/mol]
  Dispersion sSAPT0              -4.29795206 [mEh]      -2.69700575 [kcal/mol]
Total sSAPT0                    -14.70519442 [mEh]      -9.22764920 [kcal/mol]
---------------------------------------------------------------------------



ClOH-OH2-syn:
SAPT Results
---------------------------------------------------------------------------
Electrostatics               -19.61963591 [mEh]     -12.31150792 [kcal/mol]
```

```
  Elst10,r                    -20.12308410 [mEh]     -12.62742644 [kcal/mol]
  Elst12,r                      0.16510488 [mEh]       0.10360488 [kcal/mol]
  Elst13,r                      0.33834331 [mEh]       0.21231364 [kcal/mol]

Exchange                       21.30908150 [mEh]      13.37165108 [kcal/mol]
  Exch10                       18.30713091 [mEh]      11.48789856 [kcal/mol]
  Exch10(S^2)                  18.11674972 [mEh]      11.36843256 [kcal/mol]
  Exch11(S^2)                   0.13168337 [mEh]       0.08263257 [kcal/mol]
  Exch12(S^2)                   2.87026722 [mEh]       1.80111995 [kcal/mol]

Induction                      -8.13600582 [mEh]      -5.10542095 [kcal/mol]
  Ind20,r                      -9.58179728 [mEh]      -6.01266882 [kcal/mol]
  Ind30,r                     -12.99086035 [mEh]      -8.15188828 [kcal/mol]
  Ind22                        -1.52512206 [mEh]      -0.95702858 [kcal/mol]
  Exch-Ind20,r                  5.23107039 [mEh]       3.28254636 [kcal/mol]
  Exch-Ind30,r                 11.68768815 [mEh]       7.33413535 [kcal/mol]
  Exch-Ind22                    0.83262259 [mEh]       0.52247858 [kcal/mol]
  delta HF,r (2)               -3.09277947 [mEh]      -1.94074850 [kcal/mol]
  delta HF,r (3)               -1.78960727 [mEh]      -1.12299556 [kcal/mol]

Dispersion                     -6.52380194 [mEh]      -4.09374770 [kcal/mol]
  Disp20                       -6.57123698 [mEh]      -4.12351363 [kcal/mol]
  Disp30                        0.22415536 [mEh]       0.14065962 [kcal/mol]
  Disp21                        0.31101574 [mEh]       0.19516533 [kcal/mol]
  Disp22 (SDQ)                 -0.09152466 [mEh]      -0.05743259 [kcal/mol]
  Disp22 (T)                   -0.98891185 [mEh]      -0.62055158 [kcal/mol]
  Est. Disp22 (T)              -1.14802857 [mEh]      -0.72039883 [kcal/mol]
  Exch-Disp20                   1.19519109 [mEh]       0.74999376 [kcal/mol]
  Exch-Disp30                  -0.08065269 [mEh]      -0.05061033 [kcal/mol]
  Ind-Disp30                   -1.98169066 [mEh]      -1.24352972 [kcal/mol]
  Exch-Ind-Disp30               1.61896943 [mEh]       1.01591870 [kcal/mol]

tal HF                         -9.25945955 [mEh]      -5.81039883 [kcal/mol]
tal SAPT0                     -14.63550544 [mEh]      -9.18391870 [kcal/mol]
tal SAPT2                     -12.16094943 [mEh]      -7.63111130 [kcal/mol]
tal SAPT2+                    -13.08948692 [mEh]      -8.21377739 [kcal/mol]
tal SAPT2+(3)                 -12.52698825 [mEh]      -7.86080414 [kcal/mol]
tal SAPT2+3                   -12.97036217 [mEh]      -8.13902548 [kcal/mol]

ecial recipe for scaled SAPT0 (see Manual):
Electrostatics sSAPT0         -20.12308410 [mEh]     -12.62742644 [kcal/mol]
Exchange sSAPT0                18.30713091 [mEh]      11.48789856 [kcal/mol]
Induction sSAPT0               -7.27685403 [mEh]      -4.56629503 [kcal/mol]
Dispersion sSAPT0              -5.33796929 [mEh]      -3.34962644 [kcal/mol]
tal sSAPT0                    -14.43077651 [mEh]      -9.05544935 [kcal/mol]

ClOH-OH2-anti:
   SAPT Results
 --------------------------------------------------------------------------------
   Electrostatics               -18.27018138 [mEh]     -11.46471191 [kcal/mol]
     Elst10,r                   -19.01044314 [mEh]     -11.92923317 [kcal/mol]
     Elst12,r                     0.53057453 [mEh]       0.33294055 [kcal/mol]
     Elst13,r                     0.20968722 [mEh]       0.13158072 [kcal/mol]

   Exchange                      19.44473029 [mEh]      12.20175247 [kcal/mol]
     Exch10                      16.86980409 [mEh]      10.58596189 [kcal/mol]
     Exch10(S^2)                 16.70142003 [mEh]      10.48029929 [kcal/mol]
     Exch11(S^2)                  0.13388393 [mEh]       0.08401343 [kcal/mol]
     Exch12(S^2)                  2.44104227 [mEh]       1.53177715 [kcal/mol]

   Induction                     -7.46398435 [mEh]      -4.68372089 [kcal/mol]
     Ind20,r                     -8.56741753 [mEh]      -5.37613567 [kcal/mol]
     Ind30,r                    -10.61611889 [mEh]      -6.66171518 [kcal/mol]
     Ind22                       -1.19672234 [mEh]      -0.75095461 [kcal/mol]
     Exch-Ind20,r                 4.51801191 [mEh]       2.83509528 [kcal/mol]
     Exch-Ind30,r                 9.46461031 [mEh]       5.93913263 [kcal/mol]
     Exch-Ind22                   0.63108933 [mEh]       0.39601453 [kcal/mol]
     delta HF,r (2)              -2.84894572 [mEh]      -1.78774043 [kcal/mol]
     delta HF,r (3)              -1.69743714 [mEh]      -1.06515789 [kcal/mol]

   Dispersion                    -5.89360572 [mEh]      -3.69829342 [kcal/mol]
     Disp20                      -5.96079755 [mEh]      -3.74045693 [kcal/mol]
```

```
    Disp30                        0.20212028 [mEh]       0.12683239 [kcal/mol]
    Disp21                        0.29773250 [mEh]       0.18682996 [kcal/mol]
    Disp22 (SDQ)                 -0.07056772 [mEh]      -0.04428191 [kcal/mol]
    Disp22 (T)                   -0.88284834 [mEh]      -0.55399570 [kcal/mol]
    Est. Disp22 (T)              -1.02803675 [mEh]      -0.64510280 [kcal/mol]
    Exch-Disp20                   1.06257253 [mEh]       0.66677433 [kcal/mol]
    Exch-Disp30                  -0.07289586 [mEh]      -0.04574284 [kcal/mol]
    Ind-Disp30                   -1.73172695 [mEh]      -1.08667507 [kcal/mol]
    Exch-Ind-Disp30               1.40799382 [mEh]       0.88352946 [kcal/mol]

 Total HF                        -9.03899039 [mEh]      -5.67205210 [kcal/mol]
 Total SAPT0                    -13.93721541 [mEh]      -8.74573471 [kcal/mol]
 Total SAPT2                    -11.39734769 [mEh]      -7.15194365 [kcal/mol]
 Total SAPT2+                   -12.19821966 [mEh]      -7.65449840 [kcal/mol]
 Total SAPT2+(3)                -11.78641217 [mEh]      -7.39608530 [kcal/mol]
 Total SAPT2+3                  -12.18304117 [mEh]      -7.64497375 [kcal/mol]

 Special recipe for scaled SAPT0 (see Manual):
   Electrostatics sSAPT0        -19.01044314 [mEh]     -11.92923317 [kcal/mol]
   Exchange sSAPT0               16.86980409 [mEh]      10.58596189 [kcal/mol]
   Induction sSAPT0              -6.76031692 [mEh]      -4.24216291 [kcal/mol]
   Dispersion sSAPT0             -4.86576128 [mEh]      -3.05331130 [kcal/mol]
 Total sSAPT0                   -13.76671724 [mEh]      -8.63874549 [kcal/mol]
 -----------------------------------------------------------------------------



BrOH-OH2-anti:
   SAPT Results
 -----------------------------------------------------------------------------
   Electrostatics               -17.54910088 [mEh]     -11.01222752 [kcal/mol]
     Elst10,r                   -18.21642936 [mEh]     -11.43098248 [kcal/mol]
     Elst12,r                     0.41827726 [mEh]       0.26247295 [kcal/mol]
     Elst13,r                     0.24905122 [mEh]       0.15628201 [kcal/mol]

   Exchange                      18.90975202 [mEh]      11.86604903 [kcal/mol]
     Exch10                      16.28160396 [mEh]      10.21686116 [kcal/mol]
     Exch10(S^2)                 16.12471287 [mEh]      10.11841051 [kcal/mol]
     Exch11(S^2)                  0.10949047 [mEh]       0.06870631 [kcal/mol]
     Exch12(S^2)                  2.51865759 [mEh]       1.58048156 [kcal/mol]

   Induction                     -7.08326198 [mEh]      -4.44481418 [kcal/mol]
     Ind20,r                     -8.12449715 [mEh]      -5.09819914 [kcal/mol]
     Ind30,r                    -10.67969756 [mEh]      -6.70161168 [kcal/mol]
     Ind22                       -1.22499827 [mEh]      -0.76869805 [kcal/mol]
     Exch-Ind20,r                 4.30610895 [mEh]       2.70212427 [kcal/mol]
     Exch-Ind30,r                 9.57911956 [mEh]       6.01098853 [kcal/mol]
     Exch-Ind22                   0.64926800 [mEh]       0.40742184 [kcal/mol]
     delta HF,r (2)              -2.68914351 [mEh]      -1.68746310 [kcal/mol]
     delta HF,r (3)              -1.58856551 [mEh]      -0.99683995 [kcal/mol]

   Dispersion                    -5.95210861 [mEh]      -3.73500470 [kcal/mol]
     Disp20                      -6.01381137 [mEh]      -3.77372377 [kcal/mol]
     Disp30                       0.20024694 [mEh]       0.12565686 [kcal/mol]
     Disp21                       0.32312967 [mEh]       0.20276694 [kcal/mol]
     Disp22 (SDQ)                -0.08135273 [mEh]      -0.05104961 [kcal/mol]
     Disp22 (T)                  -0.92650051 [mEh]      -0.58138787 [kcal/mol]
     Est. Disp22 (T)             -1.06203256 [mEh]      -0.66643552 [kcal/mol]
     Exch-Disp20                  1.05817334 [mEh]       0.66401382 [kcal/mol]
     Exch-Disp30                 -0.07355167 [mEh]      -0.04615437 [kcal/mol]
     Ind-Disp30                  -1.66664666 [mEh]      -1.04583661 [kcal/mol]
     Exch-Ind-Disp30              1.36373643 [mEh]       0.85575757 [kcal/mol]

 Total HF                        -8.44235711 [mEh]      -5.29765929 [kcal/mol]
 Total SAPT0                    -13.39799513 [mEh]      -8.40736923 [kcal/mol]
 Total SAPT2                    -10.92730009 [mEh]      -6.85698462 [kcal/mol]
 Total SAPT2+                   -11.74755572 [mEh]      -7.37170281 [kcal/mol]
 Total SAPT2+(3)                -11.29825756 [mEh]      -7.08976395 [kcal/mol]
 Total SAPT2+3                  -11.67471946 [mEh]      -7.32599737 [kcal/mol]

 Special recipe for scaled SAPT0 (see Manual):
```

```
   Electrostatics sSAPT0         -18.21642936 [mEh]     -11.43098248 [kcal/mol]
   Exchange sSAPT0                16.28160396 [mEh]      10.21686116 [kcal/mol]
   Induction sSAPT0               -6.38061133 [mEh]      -4.00389423 [kcal/mol]
   Dispersion sSAPT0              -4.92444891 [mEh]      -3.09013847 [kcal/mol]
 Total sSAPT0                    -13.23988564 [mEh]      -8.30815402 [kcal/mol]
 ---------------------------------------------------------------------------



HOCl-OH2-anti:
   SAPT Results
 ---------------------------------------------------------------------------
   Electrostatics                 -7.68771437 [mEh]      -4.82411360 [kcal/mol]
     Elst10,r                     -7.69789216 [mEh]      -4.83050026 [kcal/mol]
     Elst12,r                     -0.48935095 [mEh]      -0.30707236 [kcal/mol]
     Elst13,r                      0.49952873 [mEh]       0.31345901 [kcal/mol]

   Exchange                       10.39201021 [mEh]       6.52108486 [kcal/mol]
     Exch10                        8.89177080 [mEh]       5.57967042 [kcal/mol]
     Exch10(S^2)                   8.84762974 [mEh]       5.55197148 [kcal/mol]
     Exch11(S^2)                   0.19296328 [mEh]       0.12108629 [kcal/mol]
     Exch12(S^2)                   1.30727613 [mEh]       0.82032816 [kcal/mol]

   Induction                      -2.63752394 [mEh]      -1.65507126 [kcal/mol]
     Ind20,r                      -6.36282305 [mEh]      -3.99273174 [kcal/mol]
     Ind30,r                     -22.51572696 [mEh]     -14.12883198 [kcal/mol]
     Ind22                        -1.38302070 [mEh]      -0.86785859 [kcal/mol]
     Exch-Ind20,r                  5.26020800 [mEh]       3.30083035 [kcal/mol]
     Exch-Ind30,r                 22.15016811 [mEh]      13.89944033 [kcal/mol]
     Exch-Ind22                    1.14335673 [mEh]       0.71746718 [kcal/mol]
     delta HF,r (2)               -1.29524492 [mEh]      -0.81277846 [kcal/mol]
     delta HF,r (3)               -0.92968607 [mEh]      -0.58338682 [kcal/mol]

   Dispersion                     -4.32376588 [mEh]      -2.71320405 [kcal/mol]
     Disp20                       -4.65225171 [mEh]      -2.91933203 [kcal/mol]
     Disp30                        0.11077033 [mEh]       0.06950943 [kcal/mol]
     Disp21                        0.50153761 [mEh]       0.31471960 [kcal/mol]
     Disp22 (SDQ)                  0.00443624 [mEh]       0.00278378 [kcal/mol]
     Disp22 (T)                   -0.72474416 [mEh]      -0.45478383 [kcal/mol]
     Est. Disp22 (T)              -0.81133739 [mEh]      -0.50912190 [kcal/mol]
     Exch-Disp20                   0.71577826 [mEh]       0.44915764 [kcal/mol]
     Exch-Disp30                  -0.05112272 [mEh]      -0.03207999 [kcal/mol]
     Ind-Disp30                   -1.16658480 [mEh]      -0.73204301 [kcal/mol]
     Exch-Ind-Disp30               1.02500830 [mEh]       0.64320242 [kcal/mol]

 Total HF                         -1.20398133 [mEh]      -0.75550969 [kcal/mol]
 Total SAPT0                      -5.14045478 [mEh]      -3.22568408 [kcal/mol]
 Total SAPT2                      -4.36923029 [mEh]      -2.74173340 [kcal/mol]
 Total SAPT2+                     -4.67459383 [mEh]      -2.93335192 [kcal/mol]
 Total SAPT2+(3)                  -4.06429477 [mEh]      -2.55038347 [kcal/mol]
 Total SAPT2+3                    -4.25699399 [mEh]      -2.67130406 [kcal/mol]

 Special recipe for scaled SAPT0 (see Manual):
   Electrostatics sSAPT0          -7.69789216 [mEh]      -4.83050026 [kcal/mol]
   Exchange sSAPT0                 8.89177080 [mEh]       5.57967042 [kcal/mol]
   Induction sSAPT0               -2.31873657 [mEh]      -1.45502917 [kcal/mol]
   Dispersion sSAPT0              -3.92570681 [mEh]      -2.46341821 [kcal/mol]
 Total sSAPT0                     -5.05056474 [mEh]      -3.16927722 [kcal/mol]
 ---------------------------------------------------------------------------

HOBr-OH2-syn:
 SAPT Results
---------------------------------------------------------------------------
 Electrostatics                -12.21748118 [mEh]      -7.66658551 [kcal/mol]
   Elst10,r                    -12.30402929 [mEh]      -7.72089527 [kcal/mol]
   Elst12,r                     -0.58328599 [mEh]      -0.36601750 [kcal/mol]
   Elst13,r                      0.66983410 [mEh]       0.42032726 [kcal/mol]

 Exchange                       16.48564472 [mEh]      10.34489867 [kcal/mol]
   Exch10                       14.14197182 [mEh]       8.87422167 [kcal/mol]
   Exch10(S^2)                  14.03758823 [mEh]       8.80871997 [kcal/mol]
```

```
   Exch11(S^2)                   0.36724334 [mEh]       0.23044868 [kcal/mol]
   Exch12(S^2)                   1.97642956 [mEh]       1.24022832 [kcal/mol]

 Induction                      -4.63172213 [mEh]      -2.90644964 [kcal/mol]
   Ind20,r                     -14.76476871 [mEh]      -9.26503263 [kcal/mol]
   Ind30,r                     -90.42935462 [mEh]     -56.74527910 [kcal/mol]
   Ind22                        -3.27042293 [mEh]      -2.05222146 [kcal/mol]
   Exch-Ind20,r                 12.58634727 [mEh]       7.89805248 [kcal/mol]
   Exch-Ind30,r                 88.95779844 [mEh]      55.82186362 [kcal/mol]
   Exch-Ind22                    2.78789865 [mEh]       1.74943289 [kcal/mol]
   delta HF,r (2)               -1.97077641 [mEh]      -1.23668092 [kcal/mol]
   delta HF,r (3)               -0.49922023 [mEh]      -0.31326544 [kcal/mol]

 Dispersion                     -5.85994726 [mEh]      -3.67717258 [kcal/mol]
   Disp20                       -6.38757678 [mEh]      -4.00826511 [kcal/mol]
   Disp30                        0.15769774 [mEh]       0.09895683 [kcal/mol]
   Disp21                        0.75544448 [mEh]       0.47404859 [kcal/mol]
   Disp22 (SDQ)                 -0.04377806 [mEh]      -0.02747115 [kcal/mol]
   Disp22 (T)                   -0.99736539 [mEh]      -0.62585626 [kcal/mol]
   Est. Disp22 (T)              -1.10592816 [mEh]      -0.69398043 [kcal/mol]
   Exch-Disp20                   1.05967255 [mEh]       0.66495459 [kcal/mol]
   Exch-Disp30                  -0.07535898 [mEh]      -0.04728848 [kcal/mol]
   Ind-Disp30                   -2.01706001 [mEh]      -1.26572432 [kcal/mol]
   Exch-Ind-Disp30               1.79693996 [mEh]       1.12759689 [kcal/mol]

otal HF                         -2.31125532 [mEh]      -1.45033467 [kcal/mol]
otal SAPT0                      -7.63915955 [mEh]      -4.79364519 [kcal/mol]
otal SAPT2                      -6.36129692 [mEh]      -3.99177425 [kcal/mol]
otal SAPT2+                     -6.75555866 [mEh]      -4.23917724 [kcal/mol]
otal SAPT2+(3)                  -5.92802682 [mEh]      -3.71989315 [kcal/mol]
otal SAPT2+3                    -6.22350586 [mEh]      -3.90530905 [kcal/mol]

pecial recipe for scaled SAPT0 (see Manual):
 Electrostatics sSAPT0         -12.30402929 [mEh]      -7.72089527 [kcal/mol]
 Exchange sSAPT0                14.14197182 [mEh]       8.87422167 [kcal/mol]
 Induction sSAPT0               -3.86632835 [mEh]      -2.42615777 [kcal/mol]
 Dispersion sSAPT0              -5.30408881 [mEh]      -3.32836612 [kcal/mol]
otal sSAPT0                     -7.33247463 [mEh]      -4.60119749 [kcal/mol]
-------------------------------------------------------------------------------



HOBr-OH2-anti:
   SAPT Results
 -------------------------------------------------------------------------------
   Electrostatics               -12.86914306 [mEh]      -8.07550953 [kcal/mol]
     Elst10,r                   -13.00064814 [mEh]      -8.15803022 [kcal/mol]
     Elst12,r                    -0.52069572 [mEh]      -0.32674151 [kcal/mol]
     Elst13,r                     0.65220080 [mEh]       0.40926220 [kcal/mol]

   Exchange                      17.08758943 [mEh]      10.72262470 [kcal/mol]
     Exch10                      14.67701099 [mEh]       9.20996383 [kcal/mol]
     Exch10(S^2)                 14.56612851 [mEh]       9.14038402 [kcal/mol]
     Exch11(S^2)                  0.37807759 [mEh]       0.23724728 [kcal/mol]
     Exch12(S^2)                  2.03250085 [mEh]       1.27541359 [kcal/mol]

   Induction                     -4.84881834 [mEh]      -3.04267957 [kcal/mol]
     Ind20,r                    -15.55546275 [mEh]      -9.76120065 [kcal/mol]
     Ind30,r                    -96.04027571 [mEh]     -60.26618539 [kcal/mol]
     Ind22                       -3.45519333 [mEh]      -2.16816664 [kcal/mol]
     Exch-Ind20,r                13.26923728 [mEh]       8.32657245 [kcal/mol]
     Exch-Ind30,r                94.44195845 [mEh]      59.26322613 [kcal/mol]
     Exch-Ind22                   2.94737488 [mEh]       1.84950573 [kcal/mol]
     delta HF,r (2)              -2.05477442 [mEh]      -1.28939047 [kcal/mol]
     delta HF,r (3)              -0.45645717 [mEh]      -0.28643121 [kcal/mol]

   Dispersion                    -5.99196617 [mEh]      -3.76001570 [kcal/mol]
     Disp20                      -6.53438291 [mEh]      -4.10038735 [kcal/mol]
     Disp30                       0.16181062 [mEh]       0.10153770 [kcal/mol]
     Disp21                       0.77319223 [mEh]       0.48518547 [kcal/mol]
     Disp22 (SDQ)                -0.04379405 [mEh]      -0.02748118 [kcal/mol]
     Disp22 (T)                  -1.01841156 [mEh]      -0.63906293 [kcal/mol]
```

```
    Est. Disp22 (T)              -1.12836873 [mEh]      -0.70806210 [kcal/mol]
    Exch-Disp20                   1.08767919 [mEh]       0.68252902 [kcal/mol]
    Exch-Disp30                  -0.07746881 [mEh]      -0.04861241 [kcal/mol]
    Ind-Disp30                   -2.09578291 [mEh]      -1.31512369 [kcal/mol]
    Exch-Ind-Disp30               1.86514919 [mEh]       1.17039884 [kcal/mol]

 Total HF                        -2.66463704 [mEh]      -1.67208506 [kcal/mol]
 Total SAPT0                     -8.11134077 [mEh]      -5.08994339 [kcal/mol]
 Total SAPT2                     -6.72927650 [mEh]      -4.22268493 [kcal/mol]
 Total SAPT2+                    -7.12824704 [mEh]      -4.47304273 [kcal/mol]
 Total SAPT2+(3)                 -6.31423562 [mEh]      -3.96224284 [kcal/mol]
 Total SAPT2+3                   -6.62233815 [mEh]      -4.15558010 [kcal/mol]

 Special recipe for scaled SAPT0 (see Manual):
   Electrostatics sSAPT0         -13.00064814 [mEh]      -8.15803022 [kcal/mol]
   Exchange sSAPT0                14.67701099 [mEh]       9.20996383 [kcal/mol]
   Induction sSAPT0               -4.03565700 [mEh]      -2.53241311 [kcal/mol]
   Dispersion sSAPT0              -5.42167477 [mEh]      -3.40215242 [kcal/mol]
 Total sSAPT0                     -7.78096893 [mEh]      -4.88263192 [kcal/mol]
 -----------------------------------------------------------------------------
```

NBO Results

FOH-OH2-syn:
 SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing: 0.50 kcal/mol
    (Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) F 1- O 2	51. RY*(1) H 3	1.13	1.55	0.037
2. BD (1) O 2- H 3	16. RY*(2) F 1	0.53	1.75	0.027
2. BD (1) O 2- H 3	93. BD*(1) F 1- O 2	1.05	0.76	0.025
6. CR (1) O 2	51. RY*(1) H 3	0.68	19.91	0.104
6. CR (1) O 2	93. BD*(1) F 1- O 2	0.82	19.08	0.112
8. LP (1) F 1	34. RY*(2) O 2	0.70	1.40	0.028
10. LP (3) F 1	33. RY*(1) O 2	0.52	1.72	0.027
10. LP (3) F 1	94. BD*(1) O 2- H 3	0.59	0.94	0.021
12. LP (2) O 2	15. RY*(1) F 1	0.99	1.31	0.032
12. LP (2) O 2	52. RY*(2) H 3	1.74	1.27	0.042
from unit 1 to unit 2				
2. BD (1) O 2- H 3	60. RY*(2) O 4	0.14	1.70	0.014
2. BD (1) O 2- H 3	61. RY*(3) O 4	0.09	1.77	0.011
12. LP (2) O 2	59. RY*(1) O 4	0.10	1.10	0.009
from unit 2 to unit 1				
3. BD (1) O 4- H 5	94. BD*(1) O 2- H 3	0.21	1.20	0.014
4. BD (1) O 4- H 6	94. BD*(1) O 2- H 3	0.21	1.20	0.014
7. CR (1) O 4	94. BD*(1) O 2- H 3	0.26	19.45	0.064
13. LP (1) O 4	94. BD*(1) O 2- H 3	0.46	0.94	0.019
14. LP (2) O 4	40. RY*(8) O 2	0.11	1.37	0.011
14. LP (2) O 4	54. RY*(4) H 3	0.19	1.46	0.015
14. LP (2) O 4	57. RY*(7) H 3	0.12	1.20	0.011
14. LP (2) O 4	94. BD*(1) O 2- H 3	18.64	0.95	0.119
within unit 2				

13. LP (1) O 4	77. RY*(1) H 5	0.91	1.59	0.034
13. LP (1) O 4	85. RY*(1) H 6	0.91	1.59	0.034

FOH-OH2-anti:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) F 1- O 2	52. RY*(2) H 3	1.32	1.58	0.041
2. BD (1) O 2- H 3	16. RY*(2) F 1	0.52	1.76	0.027
2. BD (1) O 2- H 3	93. BD*(1) F 1- O 2	1.10	0.76	0.026
6. CR (1) O 2	52. RY*(2) H 3	0.63	19.93	0.100
6. CR (1) O 2	93. BD*(1) F 1- O 2	0.84	19.08	0.113
9. LP (2) F 1	34. RY*(2) O 2	0.74	1.39	0.029
10. LP (3) F 1	33. RY*(1) O 2	0.52	1.78	0.027
10. LP (3) F 1	94. BD*(1) O 2- H 3	0.68	0.97	0.023
12. LP (2) O 2	15. RY*(1) F 1	1.02	1.30	0.032
12. LP (2) O 2	51. RY*(1) H 3	1.69	1.26	0.041
from unit 1 to unit 2				
1. BD (1) F 1- O 2	60. RY*(2) O 4	0.06	1.77	0.009
2. BD (1) O 2- H 3	60. RY*(2) O 4	0.14	1.80	0.014
2. BD (1) O 2- H 3	95. BD*(1) O 4- H 5	0.10	1.21	0.010
2. BD (1) O 2- H 3	96. BD*(1) O 4- H 6	0.10	1.21	0.010
12. LP (2) O 2	59. RY*(1) O 4	0.10	1.08	0.009
from unit 2 to unit 1				
3. BD (1) O 4- H 5	52. RY*(2) H 3	0.07	1.63	0.009
3. BD (1) O 4- H 5	94. BD*(1) O 2- H 3	0.09	1.21	0.009
4. BD (1) O 4- H 6	52. RY*(2) H 3	0.07	1.63	0.009
4. BD (1) O 4- H 6	94. BD*(1) O 2- H 3	0.09	1.21	0.009
7. CR (1) O 4	94. BD*(1) O 2- H 3	0.23	19.46	0.061
13. LP (1) O 4	94. BD*(1) O 2- H 3	0.33	0.87	0.015
14. LP (2) O 4	41. RY*(9) O 2	0.10	2.62	0.015
14. LP (2) O 4	56. RY*(6) H 3	0.17	1.63	0.015
14. LP (2) O 4	94. BD*(1) O 2- H 3	16.11	1.03	0.115
within unit 2				
13. LP (1) O 4	77. RY*(1) H 5	1.30	1.52	0.040
13. LP (1) O 4	85. RY*(1) H 6	1.30	1.52	0.040
14. LP (2) O 4	78. RY*(2) H 5	0.58	1.75	0.029
14. LP (2) O 4	86. RY*(2) H 6	0.58	1.75	0.029

ClOH-OH2-syn:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1)Cl 1- O 2	56. RY*(2) H 3	0.88	1.48	0.032
2. BD (1) O 2- H 3	20. RY*(2)Cl 1	1.21	1.41	0.037
10. CR (1) O 2	57. RY*(3) H 3	0.57	20.60	0.097
14. LP (3)Cl 1	98. BD*(1) O 2- H 3	0.78	0.84	0.023
15. LP (1) O 2	20. RY*(2)Cl 1	1.11	1.36	0.035
16. LP (2) O 2	19. RY*(1)Cl 1	4.47	0.94	0.058
16. LP (2) O 2	55. RY*(1) H 3	1.41	1.21	0.037
from unit 1 to unit 2				
2. BD (1) O 2- H 3	65. RY*(3) O 4	0.18	2.05	0.017
14. LP (3)Cl 1	64. RY*(2) O 4	0.06	1.26	0.008
16. LP (2) O 2	63. RY*(1) O 4	0.08	1.16	0.008

```
 from unit  2 to unit  1
   3. BD ( 1) O 4- H 5       98. BD*( 1) O 2- H 3         0.18    1.21    0.013
   4. BD ( 1) O 4- H 6       98. BD*( 1) O 2- H 3         0.18    1.21    0.013
  11. CR ( 1) O 4            98. BD*( 1) O 2- H 3         0.25   19.46    0.063
  17. LP ( 1) O 4            98. BD*( 1) O 2- H 3         0.49    0.95    0.019
  18. LP ( 2) O 4            39. RY*( 3) O 2              0.08    1.34    0.009
  18. LP ( 2) O 4            51. RY*(15) O 2              0.08    1.52    0.010
  18. LP ( 2) O 4            57. RY*( 3) H 3              0.05    2.09    0.010
  18. LP ( 2) O 4            58. RY*( 4) H 3              0.09    1.91    0.012
  18. LP ( 2) O 4            61. RY*( 7) H 3              0.13    1.36    0.012
  18. LP ( 2) O 4            62. RY*( 8) H 3              0.05    2.14    0.009
  18. LP ( 2) O 4            98. BD*( 1) O 2- H 3        17.75    0.96    0.116

 within unit  2
  17. LP ( 1) O 4            81. RY*( 1) H 5              0.94    1.55    0.034
  17. LP ( 1) O 4            89. RY*( 1) H 6              0.94    1.55    0.034
  18. LP ( 2) O 4            82. RY*( 2) H 5              0.55    1.61    0.027
  18. LP ( 2) O 4            90. RY*( 2) H 6              0.55    1.61    0.027

ClOH-OH2-anti:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

    Threshold for printing:   0.50 kcal/mol
   (Intermolecular threshold: 0.05 kcal/mol)
                                                            E(2)  E(j)-E(i) F(i,j
     Donor NBO (i)              Acceptor NBO (j)       kcal/mol   a.u.    a.u.
================================================================================

within unit  1
  1. BD ( 1)Cl 1- O 2       56. RY*( 2) H 3              1.23    1.47    0.038
  2. BD ( 1) O 2- H 3       20. RY*( 2)Cl 1              1.21    1.41    0.037
 10. CR ( 1) O 2            57. RY*( 3) H 3              0.78   20.47    0.113
 14. LP ( 3)Cl 1            98. BD*( 1) O 2- H 3         0.91    0.87    0.025
 15. LP ( 1) O 2            20. RY*( 2)Cl 1              1.08    1.36    0.034
 16. LP ( 2) O 2            19. RY*( 1)Cl 1              4.42    0.94    0.058
 16. LP ( 2) O 2            55. RY*( 1) H 3              1.39    1.20    0.037

from unit  1 to unit  2
  1. BD ( 1)Cl 1- O 2       66. RY*( 4) O 4              0.06    1.76    0.009
  2. BD ( 1) O 2- H 3       64. RY*( 2) O 4              0.10    1.54    0.011
  2. BD ( 1) O 2- H 3       65. RY*( 3) O 4              0.12    1.76    0.013
  2. BD ( 1) O 2- H 3       99. BD*( 1) O 4- H 5         0.06    1.21    0.008
  2. BD ( 1) O 2- H 3      100. BD*( 1) O 4- H 6         0.06    1.21    0.008
 14. LP ( 3)Cl 1            64. RY*( 2) O 4              0.05    1.21    0.007
 16. LP ( 2) O 2            63. RY*( 1) O 4              0.07    1.13    0.008

from unit  2 to unit  1
  3. BD ( 1) O 4- H 5       56. RY*( 2) H 3              0.06    1.58    0.009
  3. BD ( 1) O 4- H 5       98. BD*( 1) O 2- H 3         0.11    1.21    0.011
  4. BD ( 1) O 4- H 6       56. RY*( 2) H 3              0.06    1.58    0.009
  4. BD ( 1) O 4- H 6       98. BD*( 1) O 2- H 3         0.11    1.21    0.011
 11. CR ( 1) O 4            98. BD*( 1) O 2- H 3         0.24   19.47    0.061
 17. LP ( 1) O 4            98. BD*( 1) O 2- H 3         0.42    0.91    0.018
 18. LP ( 2) O 4            45. RY*( 9) O 2              0.06    2.55    0.011
 18. LP ( 2) O 4            61. RY*( 7) H 3              0.21    1.85    0.018
 18. LP ( 2) O 4            98. BD*( 1) O 2- H 3        16.46    1.01    0.115

within unit  2
 17. LP ( 1) O 4            81. RY*( 1) H 5              1.14    1.55    0.038
 17. LP ( 1) O 4            89. RY*( 1) H 6              1.14    1.55    0.038
 18. LP ( 2) O 4            82. RY*( 2) H 5              0.57    1.69    0.028
 18. LP ( 2) O 4            90. RY*( 2) H 6              0.57    1.69    0.028

BrOH-OH2-anti:
 SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.50 kcal/mol
    (Intermolecular threshold: 0.05 kcal/mol)
                                                            E(2)  E(j)-E(i) F(i,j
      Donor NBO (i)              Acceptor NBO (j)       kcal/mol   a.u.    a.u.
 ================================================================================
```

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1)Br 1- O 2	65. RY*(2) H 3	0.87	1.45	0.032
2. BD (1) O 2- H 3	29. RY*(2)Br 1	0.94	1.32	0.031
19. CR (1) O 2	66. RY*(3) H 3	0.81	20.35	0.115
23. LP (3)Br 1	107. BD*(1) O 2- H 3	0.65	0.86	0.021
24. LP (1) O 2	29. RY*(2)Br 1	0.78	1.28	0.028
25. LP (2) O 2	28. RY*(1)Br 1	3.46	0.84	0.048
25. LP (2) O 2	64. RY*(1) H 3	1.25	1.23	0.035
from unit 1 to unit 2				
1. BD (1)Br 1- O 2	75. RY*(4) O 4	0.05	1.73	0.008
2. BD (1) O 2- H 3	73. RY*(2) O 4	0.10	1.63	0.011
2. BD (1) O 2- H 3	74. RY*(3) O 4	0.11	1.75	0.013
23. LP (3)Br 1	73. RY*(2) O 4	0.05	1.28	0.007
25. LP (2) O 2	72. RY*(1) O 4	0.07	1.12	0.008
from unit 2 to unit 1				
3. BD (1) O 4- H 5	107. BD*(1) O 2- H 3	0.09	1.22	0.009
4. BD (1) O 4- H 6	107. BD*(1) O 2- H 3	0.09	1.22	0.009
20. CR (1) O 4	107. BD*(1) O 2- H 3	0.20	19.47	0.056
26. LP (1) O 4	107. BD*(1) O 2- H 3	0.40	0.93	0.017
27. LP (2) O 4	70. RY*(7) H 3	0.19	1.63	0.016
27. LP (2) O 4	107. BD*(1) O 2- H 3	15.31	1.01	0.111
within unit 2				
26. LP (1) O 4	90. RY*(1) H 5	1.10	1.56	0.037
26. LP (1) O 4	98. RY*(1) H 6	1.10	1.56	0.037
27. LP (2) O 4	91. RY*(2) H 5	0.55	1.68	0.027
27. LP (2) O 4	99. RY*(2) H 6	0.55	1.68	0.027

HOCl-OH2-anti:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) H 1- O 2	46. RY*(2)Cl 3	1.31	1.47	0.039
1. BD (1) H 1- O 2	98. BD*(1) O 2-Cl 3	0.52	0.76	0.018
12. LP (1) O 2	20. RY*(2) H 1	0.54	1.27	0.023
12. LP (1) O 2	46. RY*(2)Cl 3	0.50	1.47	0.024
13. LP (2) O 2	19. RY*(1) H 1	1.87	1.12	0.041
13. LP (2) O 2	45. RY*(1)Cl 3	3.81	1.02	0.056
15. LP (2)Cl 3	28. RY*(2) O 2	0.57	1.02	0.021
16. LP (3)Cl 3	27. RY*(1) O 2	0.67	1.40	0.027
16. LP (3)Cl 3	97. BD*(1) H 1- O 2	1.11	0.82	0.027
from unit 1 to unit 2				
2. BD (1) O 2-Cl 3	64. RY*(2) O 4	0.08	1.17	0.009
2. BD (1) O 2-Cl 3	65. RY*(3) O 4	0.08	1.60	0.010
2. BD (1) O 2-Cl 3	83. RY*(3) H 5	0.06	1.59	0.008
2. BD (1) O 2-Cl 3	91. RY*(3) H 6	0.06	1.59	0.008
15. LP (2)Cl 3	63. RY*(1) O 4	0.11	0.88	0.009
from unit 2 to unit 1				
17. LP (1) O 4	49. RY*(5)Cl 3	0.06	1.64	0.009
17. LP (1) O 4	98. BD*(1) O 2-Cl 3	0.19	0.59	0.009
18. LP (2) O 4	46. RY*(2)Cl 3	0.10	1.12	0.009
18. LP (2) O 4	47. RY*(3)Cl 3	0.33	1.00	0.016
18. LP (2) O 4	98. BD*(1) O 2-Cl 3	3.75	0.41	0.035
within unit 2				
17. LP (1) O 4	82. RY*(2) H 5	0.58	1.62	0.027
17. LP (1) O 4	90. RY*(2) H 6	0.58	1.62	0.027
18. LP (2) O 4	81. RY*(1) H 5	1.15	1.40	0.036

18. LP (2) O 4	89. RY*(1) H 6	1.15	1.40	0.036

HOBr-OH2-syn:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) H 1- O 2	55. RY*(2)Br 3	0.60	1.34	0.025
21. LP (1) O 2	29. RY*(2) H 1	0.57	1.26	0.024
22. LP (2) O 2	28. RY*(1) H 1	1.77	1.14	0.040
22. LP (2) O 2	54. RY*(1)Br 3	2.92	0.92	0.046
25. LP (3)Br 3	106. BD*(1) H 1- O 2	0.81	0.82	0.023
from unit 1 to unit 2				
2. BD (1) O 2-Br 3	73. RY*(2) O 4	0.22	1.14	0.014
24. LP (2)Br 3	72. RY*(1) O 4	0.13	0.88	0.010
24. LP (2)Br 3	108. BD*(1) O 4- H 5	0.06	0.75	0.006
24. LP (2)Br 3	109. BD*(1) O 4- H 6	0.06	0.75	0.006
from unit 2 to unit 1				
3. BD (1) O 4- H 5	107. BD*(1) O 2-Br 3	0.09	0.74	0.007
4. BD (1) O 4- H 6	107. BD*(1) O 2-Br 3	0.09	0.74	0.007
20. CR (1) O 4	107. BD*(1) O 2-Br 3	0.06	18.99	0.031
26. LP (1) O 4	57. RY*(4)Br 3	0.05	1.31	0.007
26. LP (1) O 4	58. RY*(5)Br 3	0.06	1.19	0.008
26. LP (1) O 4	107. BD*(1) O 2-Br 3	0.45	0.54	0.014
27. LP (2) O 4	55. RY*(2)Br 3	0.59	1.04	0.022
27. LP (2) O 4	107. BD*(1) O 2-Br 3	6.66	0.43	0.048
within unit 2				
26. LP (1) O 4	90. RY*(1) H 5	0.55	1.56	0.026
26. LP (1) O 4	98. RY*(1) H 6	0.55	1.56	0.026
27. LP (2) O 4	90. RY*(1) H 5	0.86	1.45	0.032
27. LP (2) O 4	98. RY*(1) H 6	0.86	1.45	0.032

HOBr-OH2-anti:
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) H 1- O 2	56. RY*(3)Br 3	0.83	1.35	0.030
21. LP (1) O 2	29. RY*(2) H 1	0.56	1.25	0.024
21. LP (1) O 2	56. RY*(3)Br 3	0.51	1.35	0.024
22. LP (2) O 2	28. RY*(1) H 1	1.75	1.14	0.040
22. LP (2) O 2	54. RY*(1)Br 3	2.92	0.92	0.046
25. LP (3)Br 3	106. BD*(1) H 1- O 2	0.82	0.82	0.023
from unit 1 to unit 2				
2. BD (1) O 2-Br 3	73. RY*(2) O 4	0.17	1.28	0.013
2. BD (1) O 2-Br 3	92. RY*(3) H 5	0.06	1.55	0.009
2. BD (1) O 2-Br 3	100. RY*(3) H 6	0.06	1.55	0.009
2. BD (1) O 2-Br 3	108. BD*(1) O 4- H 5	0.06	1.07	0.007
2. BD (1) O 2-Br 3	109. BD*(1) O 4- H 6	0.06	1.07	0.007
24. LP (2)Br 3	72. RY*(1) O 4	0.14	0.88	0.010
24. LP (2)Br 3	108. BD*(1) O 4- H 5	0.06	0.75	0.006
24. LP (2)Br 3	109. BD*(1) O 4- H 6	0.06	0.75	0.006
from unit 2 to unit 1				
3. BD (1) O 4- H 5	107. BD*(1) O 2-Br 3	0.10	0.74	0.008
4. BD (1) O 4- H 6	107. BD*(1) O 2-Br 3	0.10	0.74	0.008
20. CR (1) O 4	107. BD*(1) O 2-Br 3	0.07	18.99	0.032

26. LP (1) O 4	57. RY*(4)Br 3	0.06	1.05	0.007
26. LP (1) O 4	59. RY*(6)Br 3	0.05	1.14	0.007
26. LP (1) O 4	107. BD*(1) O 2-Br 3	0.47	0.55	0.014
27. LP (2) O 4	55. RY*(2)Br 3	0.63	1.01	0.023
27. LP (2) O 4	107. BD*(1) O 2-Br 3	6.98	0.43	0.049

within unit 2

26. LP (1) O 4	90. RY*(1) H 5	0.50	1.55	0.025
26. LP (1) O 4	91. RY*(2) H 5	0.50	1.60	0.025
26. LP (1) O 4	98. RY*(1) H 6	0.50	1.55	0.025
26. LP (1) O 4	99. RY*(2) H 6	0.50	1.60	0.025
27. LP (2) O 4	90. RY*(1) H 5	0.89	1.43	0.032
27. LP (2) O 4	98. RY*(1) H 6	0.89	1.43	0.032

Table 1: Harmonic vibrational frequencies in cm $^{-1}$ for all nine dimer structures. Each structure is C_S symmetry with vibrational modes in either the a$'$ or a$''$ symmetry group.

Symmetry	Number	FOH-	ClOH-	BrOH-	HOCl-	HOBr-
			syn-			
a$'$	1	3809	3805			3903
	2	3570	3582			3796
	3	1646	1646			1644
	4	1478	1382			1173
	5	913	734			622
	6	233	246			220
	7	164	193			126
	8	85	73			88
a$''$	9	3916	3911			3903
	10	701	710			272
	11	212	212			85
	12	40	24			27
			anti-			
a$'$	1	3799	3799	3802	3800	3794
	2	3523	3552	3592	3783	3786
	3	1650	1649	1647	1646	1645
	4	1499	1396	1315	1253	1174
	5	908	731	637	721	622
	6	310	295	242	205	244
	7	237	228	190	112	129
	8	83	74	63	86	91
a$''$	9	3903	3902	3906	3908	3900
	10	746	735	698	225	279
	11	227	227	206	77	86
	12	42	14	28	71	72

Table 2: Single point interaction energies based on CCSD(T)/aug-pVTZ-X2C with and without the X2C-1e method to treat relativistic effects. Energies given in kcal mol^{-1}.

Dimer	$E_{interaction}$ CCSD(T)/aug-cc-pVTZ-X2C	$E_{interaction}$ CCSD(T)/aug-cc-pVTZ
$FOH\cdots OH_2$	-8.26	-8.28
$ClOH\cdots OH_2$	-7.63	-7.67
$BrOH\cdots OH_2$	-7.27	-7.37
$HOCl\cdots OH_2$	-2.92	-2.87
$HOBr\cdots OH_2$	-4.47	–4.19