

**HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>) + CH<sub>3</sub>CH<sub>2</sub>Br/ HO<sub>w</sub><sup>-</sup>(H<sub>2</sub>O) + CH<sub>3</sub>CH<sub>2</sub>Br (B3LYP):**

**1R**

HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.24219400 | 0.09155400  | -0.06787700 |
| H | -1.56521700 | -0.57603300 | 0.55085100  |
| O | 1.23693900  | -0.09759200 | -0.05373300 |
| H | 1.48506900  | 0.65863700  | 0.49001200  |
| H | 0.12219200  | -0.03430500 | -0.06798300 |

CH<sub>3</sub>CH<sub>2</sub>Br

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.09358200 | -0.40228700 | -0.00000100 |
| H  | -2.01114300 | -1.03744200 | -0.89091400 |
| H  | -3.09120700 | 0.06466900  | 0.00021900  |
| H  | -2.01087100 | -1.03770200 | 0.89070800  |
| C  | -1.03853300 | 0.68793700  | -0.00000100 |
| H  | -1.08696000 | 1.31742800  | -0.89364800 |
| H  | -1.08693500 | 1.31741700  | 0.89365900  |
| Br | 0.80228000  | -0.06680800 | 0.00000000  |

***anti-E2***

1RC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.50288800  | 1.45902800  | 0.54201400  |
| H  | -0.01877200 | 2.34725800  | 0.15781000  |
| H  | 1.59566300  | 1.55530800  | 0.37274200  |
| H  | 0.30323300  | 1.36259800  | 1.61809600  |
| C  | 0.11112300  | 0.21131600  | -0.20441900 |
| H  | 0.26875400  | 0.29838100  | -1.28158700 |
| H  | 0.60924800  | -0.68451900 | 0.17625700  |
| Br | -1.88870700 | -0.19300200 | -0.05237900 |
| O  | 3.29952600  | 0.75926800  | -0.45824400 |
| H  | 4.24830200  | 0.93216400  | -0.47102500 |
| O  | 2.86791900  | -1.55971200 | 0.40419500  |
| H  | 3.09649100  | -0.56624000 | 0.04805200  |
| H  | 2.97820500  | -2.10837400 | -0.38025300 |

1TS(aE)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.61224300  | 0.65178700  | 0.59236600  |
| H | 0.35333600  | 1.70005300  | 0.79299600  |
| H | 1.79222500  | 0.67182500  | 0.11302500  |
| H | 0.67537700  | 0.07497100  | 1.52356100  |
| C | -0.18995300 | 0.03401600  | -0.43638000 |
| H | -0.31934200 | 0.59936100  | -1.36000600 |
| H | -0.02076900 | -1.02852800 | -0.61456500 |

|                                  |             |             |             |
|----------------------------------|-------------|-------------|-------------|
| Br                               | -2.41537500 | -0.15960300 | 0.01551600  |
| O                                | 3.11238800  | 0.70669200  | -0.36753400 |
| H                                | 3.38319800  | 1.63334900  | -0.38764400 |
| O                                | 5.19489500  | -0.79257000 | 0.23990600  |
| H                                | 4.39032300  | -0.20221500 | 0.05342100  |
| H                                | 5.29177000  | -1.29050300 | -0.57874100 |
| 1PC(aE)                          |             |             |             |
| C                                | 3.43470200  | -0.65087200 | 0.06813800  |
| H                                | 3.13343200  | -1.22178000 | 0.94880700  |
| H                                | 1.39306700  | 1.23533700  | 1.07714200  |
| H                                | 4.48373200  | -0.34964500 | 0.01082700  |
| C                                | 2.55251400  | -0.33777500 | -0.88741600 |
| H                                | 1.49982400  | -0.63008700 | -0.82168000 |
| H                                | 2.85481800  | 0.23934300  | -1.76463400 |
| Br                               | -1.26178700 | -0.88034000 | 0.01953400  |
| O                                | 0.55877900  | 1.52022800  | 1.47254200  |
| H                                | -0.05267400 | 0.78815300  | 1.21880600  |
| O                                | -0.97982500 | 2.54713200  | -0.89743800 |
| H                                | -0.42080600 | 2.52193300  | -0.10251600 |
| H                                | -1.28378400 | 1.62163800  | -0.93560000 |
| 1P1(E)                           |             |             |             |
| H <sub>2</sub> O                 |             |             |             |
| O                                | 0.00000000  | 0.00000000  | 0.11782600  |
| H                                | 0.00000000  | 0.76415700  | -0.47130400 |
| H                                | 0.00000000  | -0.76415700 | -0.47130400 |
| CH <sub>2</sub> =CH <sub>2</sub> |             |             |             |
| C                                | 0.00000000  | 0.66763200  | 0.00000000  |
| H                                | 0.92871600  | 1.24080900  | 0.00000000  |
| H                                | -0.92871600 | 1.24080900  | 0.00000000  |
| C                                | 0.00000000  | -0.66763200 | 0.00000000  |
| H                                | -0.92871600 | -1.24080900 | 0.00000000  |
| H                                | 0.92871600  | -1.24080900 | 0.00000000  |
| <i>syn-E2</i>                    |             |             |             |
| 1RC(sE)                          |             |             |             |
| C                                | -0.56845200 | 1.39071200  | -0.31544500 |
| H                                | -1.64875000 | 1.44117900  | -0.09809200 |
| H                                | -0.44768800 | 1.31160600  | -1.40400700 |
| H                                | -0.07326700 | 2.30861400  | 0.03404100  |
| C                                | -0.04732300 | 0.15378600  | 0.37741800  |
| H                                | -0.07539000 | 0.23722700  | 1.46788600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.57911500 | -0.75289800 | 0.04820500  |
| Br | 1.93688100  | -0.13090000 | -0.00236600 |
| O  | -2.45125800 | -1.44507200 | -0.27437000 |
| H  | -2.84145800 | -2.25811100 | 0.06789600  |
| O  | -3.88785500 | 0.53608800  | 0.27993900  |
| H  | -3.29717600 | -0.34236600 | 0.06660400  |
| H  | -4.42042700 | 0.64113600  | -0.51612100 |

1TS(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.40006100  | 1.78642500  | 0.14319800  |
| H  | 0.93935300  | 2.29440500  | -0.66954000 |
| H  | 1.11817800  | 0.77544100  | 0.31465800  |
| H  | 0.49325500  | 2.33898400  | 1.08850100  |
| C  | -0.99447900 | 1.52996700  | -0.21697500 |
| H  | -1.77441600 | 1.92054300  | 0.43778700  |
| H  | -1.26006800 | 1.63367600  | -1.26992700 |
| Br | -1.65006200 | -0.58895500 | -0.02881800 |
| O  | 2.03179700  | -0.28547300 | 0.53499600  |
| H  | 1.48742400  | -1.07356700 | 0.41246100  |
| O  | 4.45372000  | -0.48986200 | -0.42884900 |
| H  | 3.48609000  | -0.42067400 | -0.10920600 |
| H  | 4.94473800  | -0.55105700 | 0.39740400  |

1PC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.43558900  | -0.64887500 | -0.06829200 |
| H  | 4.48440200  | -0.34702800 | -0.01024500 |
| H  | 1.39293600  | 1.23803100  | -1.07479700 |
| H  | 3.13497800  | -1.21875800 | -0.94985000 |
| C  | 2.55287600  | -0.33771600 | 0.88741200  |
| H  | 1.50039500  | -0.63064100 | 0.82096400  |
| H  | 2.85456400  | 0.23837400  | 1.76552000  |
| Br | -1.26106700 | -0.88125500 | -0.01992500 |
| O  | 0.55865200  | 1.52211300  | -1.47078900 |
| H  | -0.05219500 | 0.78917000  | -1.21812100 |
| O  | -0.98345300 | 2.54680200  | 0.89718200  |
| H  | -0.42348300 | 2.52196700  | 0.10290900  |
| H  | -1.28663600 | 1.62103900  | 0.93514800  |

*inv-S<sub>N</sub>2*

1RC(iS)

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.56899500 | -1.38979800 | 0.31488500  |
| H | 0.44845800 | -1.31083000 | 1.40348400  |
| H | 1.64926500 | -1.43978000 | 0.09728100  |
| H | 0.07412600 | -2.30788300 | -0.03456800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.04713900  | -0.15303400 | -0.37770900 |
| H  | 0.57856100  | 0.75381500  | -0.04844000 |
| H  | 0.07503100  | -0.23627000 | -1.46820000 |
| Br | -1.93714600 | 0.13063000  | 0.00252900  |
| O  | 2.45147000  | 1.44486000  | 0.27387000  |
| H  | 2.84240100  | 2.25791200  | -0.06753200 |
| O  | 3.88833800  | -0.53634000 | -0.27945000 |
| H  | 4.41939000  | -0.64236400 | 0.51751100  |
| H  | 3.29761500  | 0.34217000  | -0.06648000 |

#### 1TS(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.60735100 | 1.24168300  | 0.16166800  |
| H  | -0.19885400 | 1.70606000  | 1.06813700  |
| H  | -1.70390600 | 1.27221900  | 0.19656300  |
| H  | -0.25686400 | 1.80933500  | -0.70938200 |
| C  | -0.19786700 | -0.19873700 | 0.06438500  |
| H  | -0.19480800 | -0.81190700 | 0.95248100  |
| H  | -0.29156800 | -0.71147300 | -0.88164500 |
| Br | 2.14564600  | -0.06959800 | -0.04922200 |
| O  | -2.38907900 | -0.90528100 | 0.20449700  |
| H  | -2.43346400 | -1.85435500 | 0.03119400  |
| O  | -4.66171400 | 0.24073700  | -0.29708300 |
| H  | -5.01900000 | 0.31521000  | 0.59430100  |
| H  | -3.76148400 | -0.23046500 | -0.14449300 |

#### 1PC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.51506600  | 0.42519900  | 0.20289500  |
| H  | 3.94826100  | 0.75510500  | -0.75299900 |
| H  | 3.66145100  | -0.66111000 | 0.28893500  |
| H  | 4.06157800  | 0.91667300  | 1.02268100  |
| C  | 2.03356600  | 0.76994900  | 0.26655000  |
| H  | 1.89798500  | 1.86581100  | 0.21065600  |
| H  | 1.60225700  | 0.43617800  | 1.22548000  |
| Br | -1.79305200 | 0.34272000  | 0.04416000  |
| O  | 1.37205900  | 0.13481000  | -0.81937300 |
| H  | 0.39973000  | 0.27407900  | -0.69800600 |
| O  | 0.31542300  | -2.50187800 | 0.11818300  |
| H  | -0.49747100 | -1.97833400 | 0.24714800  |
| H  | 0.89139700  | -1.83794100 | -0.29665000 |

#### 1P1(S)

CH<sub>3</sub>CH<sub>2</sub>OH

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.21761000 | -0.24251800 | 0.02172500  |
| H | 2.08631100 | 0.42806900  | -0.05724200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.28009700  | -0.96835200 | -0.80378100 |
| H | 1.28465500  | -0.79208500 | 0.97057000  |
| C | -0.07840100 | 0.55697300  | -0.04723700 |
| H | -0.13034900 | 1.12497700  | -0.99269100 |
| H | -0.12723300 | 1.28192900  | 0.77618800  |
| O | -1.24513300 | -0.25713400 | 0.10842300  |
| H | -1.26767400 | -0.90419900 | -0.60736000 |

*ret-S<sub>N</sub>2*

1RC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.56845800 | 1.39079300  | 0.31568800  |
| H  | -0.44760700 | 1.31161000  | 1.40423500  |
| H  | -1.64877100 | 1.44132600  | 0.09841800  |
| H  | -0.07325400 | 2.30869100  | -0.03377800 |
| C  | -0.04745300 | 0.15388500  | -0.37730200 |
| H  | -0.57927300 | -0.75280100 | -0.04812300 |
| H  | -0.07559600 | 0.23741400  | -1.46776300 |
| Br | 1.93677200  | -0.13093100 | 0.00230400  |
| O  | -2.45129800 | -1.44525500 | 0.27464400  |
| H  | -2.84114600 | -2.25800100 | -0.06871900 |
| O  | -3.88726300 | 0.53621400  | -0.28015100 |
| H  | -3.29683500 | -0.34237400 | -0.06662100 |
| H  | -4.42058600 | 0.64096900  | 0.51544300  |

1TS(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.64809000 | 2.15159900  | 0.28629700  |
| H  | -1.52578500 | 1.97106900  | 0.91028000  |
| H  | -0.76140300 | 3.09506100  | -0.28881100 |
| H  | 0.23437600  | 2.27701200  | 0.92695600  |
| C  | -0.44481300 | 1.05126500  | -0.69158600 |
| H  | -1.30498900 | 0.50059400  | -1.05051100 |
| H  | 0.36368400  | 1.18705700  | -1.40227700 |
| Br | 1.67978700  | -0.41022600 | -0.02894300 |
| O  | -1.49893400 | -0.42015200 | 0.84106700  |
| H  | -0.80643400 | -1.09158000 | 0.87509300  |
| O  | -3.66550500 | -0.97275000 | -0.44398600 |
| H  | -2.78113900 | -0.82315500 | 0.06626300  |
| H  | -4.33791100 | -0.83211500 | 0.23111200  |

1PC(rS)

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.36150600 | 0.61723200  | 1.07175200 |
| H | -2.77924800 | -0.37758600 | 1.28392900 |
| H | -3.01121700 | 1.37816800  | 1.53527200 |
| H | -1.36414400 | 0.67683200  | 1.52751400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.26405000 | 0.85011600  | -0.43577200 |
| H  | -3.26385400 | 0.79300200  | -0.89649800 |
| H  | -1.86736100 | 1.86313500  | -0.62816100 |
| Br | 1.59241300  | 0.36404100  | 0.04118900  |
| O  | -1.46407800 | -0.12041100 | -1.09792700 |
| H  | -0.51973600 | 0.05571200  | -0.85967300 |
| O  | -0.36151800 | -2.61551500 | 0.18969800  |
| H  | -0.97742000 | -2.01973000 | -0.26735400 |
| H  | 0.40662700  | -2.02765700 | 0.31331700  |

***PT***

1RC(PT)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.53785400 | 1.44864300  | 0.38182300  |
| H  | -0.40760800 | 1.33551100  | 1.46635300  |
| H  | -1.61728100 | 1.54620900  | 0.17867500  |
| H  | -0.01035300 | 2.35553600  | 0.05123500  |
| C  | -0.07413300 | 0.21147200  | -0.35102500 |
| H  | -0.62670200 | -0.68776500 | -0.03107700 |
| H  | -0.11979800 | 0.32367000  | -1.43833600 |
| Br | 1.90166400  | -0.15102400 | -0.01460000 |
| O  | -2.44078900 | -1.51583600 | 0.16784900  |
| H  | -2.82433800 | -2.06573700 | 0.86129900  |
| O  | -3.77733700 | 0.57610400  | -0.14926000 |
| H  | -4.30844500 | 0.38000900  | -0.92860700 |
| H  | -3.22678600 | -0.34443500 | 0.01796500  |

1TS(PT)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.08463900 | 2.23967100  | 0.55441700  |
| H  | -0.05941500 | 2.60161500  | -0.48521100 |
| H  | 0.67009400  | 2.82512300  | 1.11409700  |
| H  | -1.07813800 | 2.49103600  | 0.97771400  |
| C  | 0.34440000  | 0.78147300  | 0.65584800  |
| H  | 1.87394100  | 0.69268000  | -0.28875400 |
| H  | 0.16769400  | 0.44999600  | 1.69581700  |
| Br | -1.23188000 | -0.34512200 | -0.25526400 |
| O  | 2.75216100  | 0.72432900  | -0.82803300 |
| H  | 2.71184500  | -0.07629700 | -1.36427000 |
| O  | 1.60466500  | -2.17440600 | 0.69327000  |
| H  | 0.68186400  | -2.22325900 | 0.40242400  |
| H  | 1.73474300  | -1.20788000 | 0.69893100  |

1PC(PT)

|   |            |            |             |
|---|------------|------------|-------------|
| C | 0.16328100 | 2.10122400 | 0.46647000  |
| H | 0.31836300 | 2.36450200 | -0.59146000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.97058000  | 2.59457300  | 1.04043300  |
| H  | -0.79599100 | 2.55339200  | 0.78845700  |
| C  | 0.30680900  | 0.60178400  | 0.71045600  |
| H  | 2.00469500  | 0.57076000  | -0.37421700 |
| H  | 0.01134200  | 0.40854000  | 1.75845500  |
| Br | -1.38381700 | -0.29535200 | -0.22443800 |
| O  | 2.86078900  | 0.56533300  | -0.88332500 |
| H  | 3.12651500  | -0.35613300 | -0.76347300 |
| O  | 1.81915300  | -1.89128000 | 0.64405500  |
| H  | 1.15377100  | -2.42647100 | 0.19581000  |
| H  | 1.38423400  | -0.98232300 | 0.65393900  |

1P1(PT)

CH<sub>3</sub>CHBr<sup>-</sup>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.12917500  | -0.37743400 | 0.02190100  |
| H  | 2.11917400  | -1.07515700 | -0.83254200 |
| H  | 3.14957100  | 0.05591100  | 0.06558300  |
| H  | 1.99329800  | -0.98749500 | 0.94530400  |
| C  | 1.18894100  | 0.80679100  | -0.19696400 |
| H  | 1.15492600  | 1.36250700  | 0.76594800  |
| Br | -0.80930500 | -0.05519700 | 0.00303100  |

***Dits***

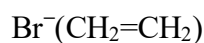
1TS(Dits)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.43504000  | 1.84165900  | 0.03634900  |
| H  | 1.13574500  | 1.38657200  | -0.71546200 |
| H  | -0.13163200 | 2.61319800  | -0.52949300 |
| H  | 1.06920500  | 2.39109000  | 0.75550600  |
| C  | -0.41834200 | 0.90773100  | 0.82088100  |
| H  | -0.26361700 | 0.55764100  | 1.83485700  |
| H  | 0.98549300  | -0.44922400 | 0.85244000  |
| Br | -1.58344900 | -0.30138700 | -0.22720100 |
| O  | 1.67770000  | -1.18593200 | 0.75119400  |
| H  | 1.21528700  | -1.81571300 | 0.18533200  |
| O  | 3.90479400  | -0.15165200 | -0.56799300 |
| H  | 3.49550500  | 0.62457100  | -0.96910300 |
| H  | 3.15459900  | -0.55524800 | -0.07104400 |

Complex

Br<sup>-</sup>(H<sub>2</sub>O)

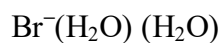
|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | -0.72445100 | 0.00230800  | -0.00000300 |
| O  | 2.62915300  | -0.08912000 | -0.00003600 |
| H  | 2.66905100  | 0.87407200  | 0.00006000  |
| H  | 1.65352900  | -0.24188200 | 0.00032400  |



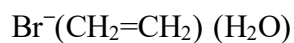
|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | 1.36030200  | -0.02658800 | -0.00002100 |
| C  | -2.51057100 | 0.53849400  | 0.00017500  |
| H  | -2.80282700 | 1.59270900  | -0.00034600 |
| H  | -1.43485200 | 0.32472400  | 0.00082900  |
| C  | -3.43997300 | -0.42322500 | -0.00006100 |
| H  | -3.15903000 | -1.47883900 | 0.00042800  |
| H  | -4.51059600 | -0.19963400 | -0.00087000 |



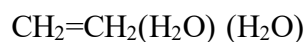
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.42342900 | -0.04989100 | 0.00034000  |
| H | -2.96719500 | -0.25975100 | -0.76842900 |
| H | -2.97620300 | -0.26400700 | 0.76147000  |
| C | 2.01966300  | -0.44757200 | -0.00032300 |
| H | 3.09798500  | -0.27733200 | -0.00340800 |
| H | 1.68923200  | -1.48802600 | 0.00178800  |
| C | 1.14582200  | 0.56303000  | 0.00085300  |
| H | 0.06765000  | 0.39388000  | 0.00393500  |
| H | 1.48305400  | 1.60162200  | -0.00125800 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | 1.09047300  | -0.04833000 | 0.00145800  |
| O  | -2.18347000 | -1.44875600 | 0.01011800  |
| H  | -2.37041300 | -0.49999000 | -0.08706400 |
| H  | -1.20875200 | -1.43783800 | 0.03669800  |
| O  | -1.80230600 | 1.54082000  | -0.09004200 |
| H  | -1.80345400 | 1.73547800  | 0.85488400  |
| H  | -0.89773300 | 1.15738100  | -0.21614300 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | 1.45723100  | -0.31731700 | -0.00762500 |
| C  | -2.46582700 | -1.25554800 | 0.06721400  |
| H  | -2.90635500 | -2.25197700 | 0.16784300  |
| H  | -1.37404400 | -1.18264800 | 0.07965900  |
| C  | -3.23408800 | -0.16941800 | -0.06903100 |
| H  | -2.78397000 | 0.82088600  | -0.16965300 |
| H  | -4.32602400 | -0.23572700 | -0.08527100 |
| O  | -0.61287900 | 2.31364600  | -0.05020100 |
| H  | -0.01062400 | 1.54739000  | -0.21099100 |
| H  | -0.49955600 | 2.44878300  | 0.89779800  |



|   |             |            |            |
|---|-------------|------------|------------|
| C | -2.07623100 | 0.02042400 | 0.48012900 |
| H | -1.69041000 | 0.02657600 | 1.50130300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.97974900 | -0.56524900 | 0.30135700  |
| C | -1.48044700 | 0.71516900  | -0.49665400 |
| H | -1.87986900 | 0.71803000  | -1.51275100 |
| H | -0.57930500 | 1.30446700  | -0.31659100 |
| O | 1.96148800  | 1.08800400  | 0.07776600  |
| H | 1.78097000  | 0.12999900  | 0.08405600  |
| H | 2.75303200  | 1.20343500  | 0.61469300  |
| O | 0.89889600  | -1.57392100 | -0.03085300 |
| H | 1.05718900  | -2.11124700 | -0.81622800 |
| H | -0.00486400 | -1.23222700 | -0.13200100 |

Br<sup>-</sup>(CH<sub>3</sub>CH<sub>2</sub>OH)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.57925600 | 0.17847800  | 0.01029700  |
| H  | -3.87715600 | -0.37498600 | 0.91340300  |
| H  | -3.89867100 | -0.40520200 | -0.86608900 |
| H  | -4.10965000 | 1.14373500  | 0.00019700  |
| C  | -2.07063000 | 0.39086100  | -0.01200300 |
| H  | -1.78350100 | 0.96823400  | -0.91078600 |
| H  | -1.75964300 | 0.99067400  | 0.86355800  |
| O  | -1.43740500 | -0.87367000 | -0.00411300 |
| H  | -0.46175700 | -0.71795300 | -0.00472500 |
| Br | 1.75111200  | 0.05625200  | 0.00135900  |

CH<sub>3</sub>CH<sub>2</sub>OH(H<sub>2</sub>O)

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.79320100 | 0.17635000  | -0.00046700 |
| H | -3.22411500 | -0.22334300 | -0.76645900 |
| H | -3.22538000 | -0.22093300 | 0.76602900  |
| C | 2.35413600  | -0.06789100 | -0.00060200 |
| H | 2.52227000  | -0.68919000 | -0.89114900 |
| H | 2.52333500  | -0.68963400 | 0.88943400  |
| H | 3.08935000  | 0.74965500  | -0.00083500 |
| C | 0.94034700  | 0.48917200  | 0.00038400  |
| H | 0.78450300  | 1.12358000  | 0.89169100  |
| H | 0.78338300  | 1.12390900  | -0.89048700 |
| O | 0.02601400  | -0.60597000 | 0.00075900  |
| H | -0.88274100 | -0.26476700 | 0.00074000  |

CH<sub>3</sub>CHBr<sup>-</sup>(H<sub>2</sub>O)

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 0.72207900  | 0.62298600 | 0.51065400  |
| H | 0.47061400  | 0.81702900 | 1.57080000  |
| C | 0.71732500  | 1.95451900 | -0.22855400 |
| H | 1.60614800  | 2.51227300 | 0.12625500  |
| H | 0.84117200  | 1.81696400 | -1.31498500 |
| H | -0.16632900 | 2.60840500 | -0.07220300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | -1.09743600 | -0.34816500 | -0.03297000 |
| O  | 2.82738000  | -1.08903900 | -0.07471900 |
| H  | 2.02368100  | -0.44649200 | 0.15788200  |
| H  | 2.37950800  | -1.87512200 | -0.40866300 |

(H<sub>2</sub>O) (H<sub>2</sub>O)

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.38749200  | 0.00117800  | 0.11112000  |
| H | 1.74443300  | -0.76986500 | -0.34742100 |
| H | 1.74307100  | 0.76295100  | -0.36366900 |
| O | -1.51406700 | -0.00157200 | -0.12179700 |
| H | -1.91944300 | 0.00984100  | 0.75244200  |
| H | -0.55546300 | 0.00023000  | 0.04406800  |

**HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)<sub>2</sub> + CH<sub>3</sub>CH<sub>2</sub>Br (B3LYP):**

**2R**

HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.00000600 | 0.65359000  | -0.01506900 |
| H | 0.00010400  | 1.44273800  | 0.53931000  |
| O | -2.39113400 | -0.29744300 | -0.07849800 |
| H | -2.29559400 | -1.06515200 | 0.49517600  |
| H | -1.43384800 | 0.10875600  | -0.07640100 |
| O | 2.39097400  | -0.29769500 | -0.07897600 |
| H | 2.29701200  | -1.06241300 | 0.49896100  |
| H | 1.43365500  | 0.10844900  | -0.07669900 |

***anti-E2***

2RC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.06495700  | 0.00004300  | 1.66169300  |
| H  | -0.34256600 | 0.89536000  | 2.15069100  |
| H  | 1.16528100  | 0.00003300  | 1.75044000  |
| H  | -0.34260100 | -0.89517400 | 2.15082100  |
| C  | -0.21344400 | -0.00005200 | 0.17828800  |
| H  | 0.16438900  | 0.89830900  | -0.31589400 |
| H  | 0.16430400  | -0.89851100 | -0.31577500 |
| Br | -2.20860900 | -0.00001100 | -0.22008400 |
| O  | 3.05682400  | 0.00003600  | 0.49127300  |
| H  | 3.97216300  | 0.00000300  | 0.79182000  |
| O  | 2.39731600  | 2.22773500  | -0.62771600 |
| H  | 2.60363200  | 2.06994200  | -1.55522400 |
| H  | 2.69568200  | 1.35348600  | -0.16285300 |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| O             | 2.39743600  | -2.22773100 | -0.62767800 |
| H             | 2.69570300  | -1.35344400 | -0.16281500 |
| H             | 2.60365300  | -2.06988000 | -1.55519900 |
| 2TS(aE)       |             |             |             |
| C             | 0.03809400  | -0.13999200 | -1.17386200 |
| H             | -0.34463200 | -0.47733300 | -2.14524200 |
| H             | 1.32385000  | -0.49787900 | -1.18222100 |
| H             | 0.05881900  | 0.95345100  | -1.09616300 |
| C             | -0.51082300 | -0.81733300 | -0.04302300 |
| H             | -0.61563200 | -1.90040200 | -0.10437600 |
| H             | -0.22536400 | -0.46188000 | 0.94674000  |
| Br            | -2.80989700 | -0.48310200 | 0.33995200  |
| O             | 2.61007600  | -0.78772000 | -1.27083500 |
| H             | 2.83736300  | -0.70020100 | -2.20485100 |
| O             | 3.69646700  | -3.02234200 | -0.20464800 |
| H             | 3.05814600  | -3.28703800 | 0.46666700  |
| H             | 3.26574900  | -2.23582600 | -0.64584900 |
| O             | 4.71570300  | 0.07425200  | 0.30505900  |
| H             | 3.92867900  | -0.07357600 | -0.27499100 |
| H             | 4.95502100  | -0.83353700 | 0.53269600  |
| 2PC(aE)       |             |             |             |
| C             | -3.28767100 | 1.91133700  | -0.23457000 |
| H             | -3.12921900 | 1.55871700  | -1.25562400 |
| H             | -0.38749000 | 1.94312200  | -0.31316900 |
| H             | -3.82395300 | 2.85590400  | -0.11585300 |
| C             | -2.84243000 | 1.21133400  | 0.81469100  |
| H             | -2.29735500 | 0.27099700  | 0.69010600  |
| H             | -3.00065800 | 1.56729600  | 1.83569400  |
| Br            | -0.26251900 | -1.65076100 | -0.23336400 |
| O             | 0.47039100  | 1.55006700  | -0.51586600 |
| H             | 0.27157500  | 0.58229400  | -0.57623400 |
| O             | 2.23599800  | 0.01573800  | 1.48257700  |
| H             | 1.71623300  | -0.72260300 | 1.10513200  |
| H             | 1.66717500  | 0.76976000  | 1.26471600  |
| O             | 3.42647500  | 1.83144500  | -0.61222000 |
| H             | 2.48103300  | 1.94060600  | -0.80723100 |
| H             | 3.40850400  | 1.09650100  | 0.02353800  |
| <i>syn-E2</i> |             |             |             |
| 2RC(sE)       |             |             |             |
| C             | -0.19271100 | -1.24131200 | 0.63096200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.17651100  | -2.19599700 | 0.23234000  |
| H  | -1.28546600 | -1.20946700 | 0.51018300  |
| H  | 0.05723600  | -1.18354200 | 1.69902700  |
| C  | 0.36490300  | -0.06407200 | -0.13270900 |
| H  | 0.12601300  | -0.10102400 | -1.19604300 |
| H  | 0.06334700  | 0.90062600  | 0.28094300  |
| Br | 2.40051800  | -0.04080000 | -0.06806900 |
| O  | -2.63020800 | 0.39672000  | -0.89545100 |
| H  | -3.05218600 | 0.71482900  | -1.70161100 |
| O  | -1.86551000 | 2.38914700  | 0.53549600  |
| H  | -2.49909700 | 2.40368200  | 1.26060200  |
| H  | -2.19534700 | 1.60735000  | -0.06344100 |
| O  | -4.05403900 | -1.51720700 | 0.09829000  |
| H  | -3.49781800 | -0.75870100 | -0.32858400 |
| H  | -4.54641900 | -1.06674700 | 0.79280700  |

#### 2TS(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.13555700 | -1.91077300 | -0.25221200 |
| H  | 0.63785700  | -0.91319500 | -0.06626900 |
| H  | 0.22137600  | -2.27853900 | -1.22321100 |
| H  | 0.15447200  | -2.56876000 | 0.57732000  |
| C  | -1.54510100 | -1.58342800 | -0.25291900 |
| H  | -2.08328300 | -1.60451600 | -1.19985400 |
| H  | -2.15643300 | -1.90835800 | 0.58813800  |
| Br | -2.03788700 | 0.63781800  | 0.10834700  |
| O  | 1.52683700  | 0.11367600  | 0.12888900  |
| H  | 0.92352200  | 0.85547200  | 0.26667300  |
| O  | 3.47397500  | 0.53762300  | -1.65302400 |
| H  | 3.49459700  | 1.49564100  | -1.75026900 |
| H  | 2.69526900  | 0.38013900  | -1.03530800 |
| O  | 3.78557200  | -0.01453000 | 1.64676400  |
| H  | 2.88195900  | 0.02415000  | 1.23331100  |
| H  | 4.34960700  | 0.06540800  | 0.86709500  |

#### 2PC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.79197200 | 2.24978700  | 0.65584200  |
| H  | -0.27947100 | 1.85861200  | -0.73621400 |
| H  | -2.09949800 | 2.09154000  | 1.48489400  |
| H  | -3.29813200 | 3.21720100  | 0.61312300  |
| C  | -3.00463200 | 1.29698700  | -0.25852700 |
| H  | -2.48989100 | 0.33257500  | -0.21612500 |
| H  | -3.69808300 | 1.45868300  | -1.08762900 |
| Br | -0.34228600 | -1.68656700 | -0.12509500 |
| O  | 0.57006100  | 1.40434700  | -0.79534100 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 0.32464100 | 0.44656000  | -0.73868300 |
| O | 2.03768800 | 0.18813600  | 1.57490200  |
| H | 1.53940800 | -0.60087600 | 1.28235300  |
| H | 1.53133600 | 0.89287900  | 1.14147300  |
| O | 3.53987800 | 1.58231700  | -0.64192400 |
| H | 2.62540000 | 1.68395500  | -0.95319400 |
| H | 3.42290500 | 0.96967700  | 0.10333800  |

*inv-S<sub>N</sub>2*

2RC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.13973300  | -1.28393100 | 1.15087500  |
| H  | 0.89103800  | -2.00078600 | 1.51178600  |
| H  | -0.82676000 | -1.79609000 | 1.01589800  |
| H  | 0.00569800  | -0.49670700 | 1.90407300  |
| C  | 0.50755700  | -0.69481900 | -0.19179800 |
| H  | 0.70276700  | -1.46172300 | -0.94702300 |
| H  | -0.25346000 | 0.01255800  | -0.55227100 |
| Br | 2.25988900  | 0.32478100  | -0.10298500 |
| O  | -2.30808200 | 0.36782300  | -0.87735000 |
| H  | -2.55690400 | 0.55857700  | -1.78922700 |
| O  | -3.35370500 | 2.23336400  | 0.61541200  |
| H  | -2.56989300 | 2.72726800  | 0.87882000  |
| H  | -2.97077300 | 1.49076500  | 0.01914000  |
| O  | -2.95699100 | -2.04346200 | -0.23429000 |
| H  | -3.74148100 | -1.90826400 | 0.30827500  |
| H  | -2.70988500 | -1.08222600 | -0.52964600 |

2TS(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.20606800 | -0.31541700 | 1.29704300  |
| H  | 0.28054100  | -1.23824000 | 1.63321800  |
| H  | -1.29168600 | -0.42614700 | 1.41352000  |
| H  | 0.14522200  | 0.51194600  | 1.92540200  |
| C  | 0.09413800  | -0.05371100 | -0.14947800 |
| H  | 0.11746300  | -0.87153400 | -0.85345100 |
| H  | 0.07644400  | 0.94988100  | -0.54382100 |
| Br | 2.52392500  | 0.01210000  | -0.10674800 |
| O  | -2.03829700 | 0.03005400  | -0.74919600 |
| H  | -2.02357300 | 0.09179600  | -1.71281000 |
| O  | -3.36139500 | 2.17348400  | 0.12671600  |
| H  | -2.68426100 | 2.67532600  | 0.59274900  |
| H  | -2.86864000 | 1.36307100  | -0.21651000 |
| O  | -3.60661700 | -2.01088500 | -0.04461300 |
| H  | -4.37622300 | -1.53487800 | 0.28609800  |
| H  | -2.99061300 | -1.27119300 | -0.33687700 |

## 2PC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.58599800 | -0.84139700 | -0.24205200 |
| H  | -4.11241500 | -1.34320300 | -1.06852300 |
| H  | -3.83228600 | 0.22938600  | -0.27056200 |
| H  | -3.95306800 | -1.25506700 | 0.70870000  |
| C  | -2.08318700 | -1.04487800 | -0.36879200 |
| H  | -1.72251700 | -0.63572400 | -1.32800300 |
| H  | -1.83910000 | -2.12187700 | -0.35879700 |
| Br | 1.76760200  | -0.80047700 | 0.01918700  |
| O  | -1.44358000 | -0.38893300 | 0.72101900  |
| H  | -0.47035200 | -0.51893500 | 0.62012600  |
| O  | 1.35124800  | 2.46909500  | -0.41819600 |
| H  | 1.47850900  | 1.48983500  | -0.44154400 |
| H  | 1.72662400  | 2.70126200  | 0.43962500  |
| O  | -1.52655700 | 2.49938300  | 0.23131700  |
| H  | -0.60286400 | 2.59359800  | -0.06627500 |
| H  | -1.57235500 | 1.55872000  | 0.48564800  |

*ret-S<sub>N</sub>2*

## 2RC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.14093300  | -1.28557200 | 1.15035100  |
| H  | 0.00708300  | -0.49924000 | 1.90451100  |
| H  | 0.89267300  | -2.00258500 | 1.51003500  |
| H  | -0.82546300 | -1.79790600 | 1.01532800  |
| C  | 0.50779700  | -0.69486200 | -0.19188300 |
| H  | 0.70296300  | -1.46089900 | -0.94799500 |
| H  | -0.25371300 | 0.01253800  | -0.55127900 |
| Br | 2.25970400  | 0.32545300  | -0.10293500 |
| O  | -2.30824600 | 0.36777200  | -0.87640900 |
| H  | -2.55613600 | 0.55858800  | -1.78852800 |
| O  | -3.35538900 | 2.23340500  | 0.61521400  |
| H  | -2.57177700 | 2.72690200  | 0.87997800  |
| H  | -2.97185100 | 1.49074700  | 0.01942400  |
| O  | -2.95576000 | -2.04415900 | -0.23462900 |
| H  | -2.70922200 | -1.08258800 | -0.52944200 |
| H  | -3.74142900 | -1.90995600 | 0.30647000  |

## 2TS(rS)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.94791400 | 0.03340500  | -1.98664300 |
| H | -0.36634700 | -0.89809500 | -1.94291600 |
| H | -0.85395200 | 0.42198200  | -3.01968400 |
| H | -1.98689100 | -0.21034200 | -1.74847600 |
| C | -0.40188300 | 1.04599800  | -1.05486600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.50695800  | 1.55186800  | -1.35918200 |
| H  | -1.07257100 | 1.60827200  | -0.41692100 |
| Br | 1.83982900  | 0.30606500  | 0.31865000  |
| O  | -1.37195400 | -0.24319900 | 0.68157700  |
| H  | -0.71182300 | -0.00749100 | 1.34571900  |
| O  | -0.44930500 | -2.66917700 | -0.03368000 |
| H  | 0.48896900  | -2.45648000 | 0.05725400  |
| H  | -0.87430600 | -1.80983600 | 0.25835200  |
| O  | -3.71726100 | 0.90691600  | 0.85082400  |
| H  | -2.80265600 | 0.46404000  | 0.84018500  |
| H  | -4.31443500 | 0.19107600  | 1.09221000  |

#### 2PC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.61835500 | -0.00011100 | -0.45350300 |
| H  | -3.86320400 | -0.89072600 | 0.14291900  |
| H  | -4.24843600 | -0.00021800 | -1.35595400 |
| H  | -3.86372100 | 0.89025800  | 0.14307200  |
| C  | -2.14475200 | 0.00035600  | -0.83220900 |
| H  | -1.90573600 | -0.88919500 | -1.44030300 |
| H  | -1.90630900 | 0.89010300  | -1.44025000 |
| Br | 1.79525500  | -0.00030200 | -0.39677600 |
| O  | -1.36844700 | 0.00055900  | 0.36222500  |
| H  | -0.41023500 | 0.00038600  | 0.10372900  |
| O  | -0.06597500 | -2.62636100 | 1.17052800  |
| H  | 0.70663200  | -2.16948100 | 0.79151700  |
| H  | -0.73942500 | -1.92975800 | 1.12108700  |
| O  | -0.06480000 | 2.62677100  | 1.17018900  |
| H  | -0.73866000 | 1.93057400  | 1.12079200  |
| H  | 0.70759800  | 2.16942700  | 0.79128200  |

#### HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)<sub>3</sub> + CH<sub>3</sub>CH<sub>2</sub>Br (B3LYP):

##### 3R

##### HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)<sub>3</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.00524700  | -0.00087200 | 0.65450800  |
| H | 0.00551500  | -0.00088700 | 1.61855600  |
| O | 2.48082500  | -0.20021000 | -0.21823200 |
| H | 2.56066000  | 0.63045600  | -0.69959300 |
| H | 1.53127300  | -0.15563400 | 0.14578500  |
| O | -1.41728700 | -2.03764100 | -0.21664900 |
| H | -0.73925800 | -2.53031900 | -0.69171100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.89901500 | -1.24036600 | 0.14647100  |
| O | -1.06905500 | 2.23984500  | -0.21580100 |
| H | -1.82746200 | 1.89129000  | -0.69695300 |
| H | -0.62955300 | 1.39648200  | 0.14683900  |

***anti-E2***

**3RC(aE)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.67016900  | 0.03514400  | 1.70247300  |
| H  | 1.13360400  | -0.85259200 | 2.15220600  |
| H  | -0.40155200 | 0.04151200  | 1.95180300  |
| H  | 1.13544100  | 0.93940600  | 2.11586200  |
| C  | 0.75643200  | 0.00435800  | 0.19420000  |
| H  | 0.31794100  | -0.90469600 | -0.22396800 |
| H  | 0.32041500  | 0.89686200  | -0.26046700 |
| Br | 2.68064100  | -0.01053900 | -0.44031800 |
| O  | -2.81496200 | 0.01707100  | 0.72460700  |
| H  | -3.32625900 | 0.03056100  | 1.54150400  |
| O  | -1.69257800 | -2.31443100 | 0.30099000  |
| H  | -2.12720000 | -1.41847800 | 0.50640200  |
| H  | -2.31443900 | -2.72559800 | -0.30891600 |
| O  | -1.68576800 | 2.32979800  | 0.23798200  |
| H  | -2.12554600 | 1.44052300  | 0.46474900  |
| H  | -2.32444100 | 2.75044300  | -0.34740200 |
| O  | -4.43421700 | -0.03997900 | -1.37829200 |
| H  | -3.85614800 | -0.01839500 | -0.54702900 |
| H  | -3.79367100 | 0.01261900  | -2.09594200 |

**3TS(aE)**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.32206200 | -0.00801800 | -1.19230100 |
| H  | -0.46972400 | -0.92684700 | -1.77067300 |
| H  | 1.04193000  | -0.00383100 | -0.94287900 |
| H  | -0.47249200 | 0.90085600  | -1.78553000 |
| C  | -0.88138700 | 0.00179900  | 0.10779300  |
| H  | -0.82919900 | -0.90855000 | 0.70266200  |
| H  | -0.83145400 | 0.92175000  | 0.68785700  |
| Br | -3.30906000 | -0.00008700 | 0.21887000  |
| O  | 2.30031700  | -0.00103100 | -0.82105500 |
| H  | 2.65898900  | -0.00175800 | -1.71820600 |
| O  | 3.17301600  | -2.68531900 | -0.15391100 |
| H  | 2.72869700  | -1.86340700 | -0.44807000 |
| H  | 3.83050400  | -2.34132600 | 0.46535700  |
| O  | 3.16348300  | 2.68767200  | -0.16010800 |
| H  | 2.72215100  | 1.86353200  | -0.45249700 |
| H  | 3.82242100  | 2.34736000  | 0.45966100  |

|   |            |            |            |
|---|------------|------------|------------|
| O | 4.09463000 | 0.00435000 | 1.27154200 |
| H | 3.46204100 | 0.00231100 | 0.50962100 |
| H | 3.52237000 | 0.00491100 | 2.04755800 |

3PC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.48407600 | 1.54915700  | 0.41535000  |
| H  | -4.13329300 | 2.42066300  | 0.30236800  |
| H  | -0.89394200 | 2.16732500  | -0.04056000 |
| H  | -3.16769600 | 1.29925500  | 1.42999000  |
| C  | -3.08901100 | 0.81674700  | -0.63233300 |
| H  | -3.40628500 | 1.07207200  | -1.64650200 |
| H  | -2.42949000 | -0.04894200 | -0.51657000 |
| Br | -0.24651000 | -1.81612000 | 0.05045200  |
| O  | 0.03471100  | 2.43516900  | -0.00070400 |
| H  | 0.41779700  | 1.87032300  | 0.71491400  |
| O  | 3.57396100  | 0.90549800  | -0.04990400 |
| H  | 3.71072600  | 1.85752200  | -0.11639500 |
| H  | 2.87105400  | 0.71852000  | -0.72504500 |
| O  | 1.25921800  | 0.67533400  | 1.76866400  |
| H  | 0.81869500  | -0.13950300 | 1.43636100  |
| H  | 2.13343600  | 0.65477400  | 1.33586800  |
| O  | 1.41765500  | 0.54722400  | -1.71284000 |
| H  | 0.88247100  | 1.25698600  | -1.30407000 |
| H  | 0.97854900  | -0.26601500 | -1.37599500 |

*syn-E2*

3RC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.49769500 | -1.09412400 | -0.14352500 |
| H  | -0.67389900 | -1.59389400 | 0.81793800  |
| H  | 0.58466200  | -0.90204100 | -0.24344200 |
| H  | -0.81878600 | -1.76359400 | -0.95293700 |
| C  | -1.20695300 | 0.23802600  | -0.20719700 |
| H  | -0.89997800 | 0.92112200  | 0.58665500  |
| H  | -1.09649200 | 0.73350300  | -1.17489100 |
| Br | -3.21061500 | 0.03884100  | 0.00531800  |
| O  | 2.77271900  | 0.01523300  | -0.55674000 |
| H  | 2.62251500  | -0.00802000 | -1.50887100 |
| O  | 3.53417400  | -2.32042900 | 0.41772000  |
| H  | 3.24110000  | -1.44245500 | 0.00592700  |
| H  | 3.12723100  | -2.30354200 | 1.29059500  |
| O  | 1.35487600  | 1.84041000  | 0.66802500  |
| H  | 1.89085300  | 1.13009600  | 0.17288100  |
| H  | 2.02795300  | 2.47314400  | 0.94006200  |
| O  | 5.17328900  | 1.13896200  | -0.24611600 |

|         |             |             |             |
|---------|-------------|-------------|-------------|
| H       | 4.25361300  | 0.75027400  | -0.39272000 |
| H       | 5.66018800  | 0.38915800  | 0.11390500  |
| 3TS(sE) |             |             |             |
| C       | 0.37584400  | -1.65041200 | 0.96358500  |
| H       | 0.05620400  | -1.60886400 | 2.01226100  |
| H       | -0.02009100 | -2.51730600 | 0.42066900  |
| H       | -0.35288200 | -0.70750500 | 0.43999100  |
| C       | 1.78064200  | -1.43100800 | 0.77369600  |
| H       | 2.39751900  | -1.14653600 | 1.62381100  |
| H       | 2.31193900  | -2.01191600 | 0.02231000  |
| Br      | 2.34152300  | 0.59051800  | -0.33682000 |
| O       | -1.14018000 | 0.23422000  | -0.09163100 |
| H       | -0.44732300 | 0.82816500  | -0.41436200 |
| O       | -2.68141800 | 0.80275600  | 2.06991300  |
| H       | -2.03023100 | 0.66545500  | 1.32659900  |
| H       | -2.88741700 | -0.09409500 | 2.35628700  |
| O       | -2.65686500 | -1.64579000 | -1.59386400 |
| H       | -1.97458000 | -1.08279900 | -1.16792700 |
| H       | -3.43121200 | -1.06694000 | -1.55067200 |
| O       | -3.74283900 | 1.15989100  | -0.77710400 |
| H       | -2.78927700 | 0.92767000  | -0.72833900 |
| H       | -3.95443600 | 1.22643800  | 0.16585700  |

|         |             |             |             |
|---------|-------------|-------------|-------------|
| 3PC(sE) |             |             |             |
| C       | -3.53205200 | 1.98648000  | 0.45944300  |
| H       | -3.06084200 | 1.79833100  | 1.42612400  |
| H       | -4.08316500 | 2.92378200  | 0.35306200  |
| H       | -0.77235800 | 1.88598300  | -0.27372600 |
| C       | -3.43508400 | 1.10387200  | -0.54096400 |
| H       | -2.87518200 | 0.17046500  | -0.43404300 |
| H       | -3.90738400 | 1.29514000  | -1.50754300 |
| Br      | -0.62913900 | -1.69088800 | 0.05800700  |
| O       | 0.09768900  | 1.47505200  | -0.19658300 |
| H       | -0.11074800 | 0.50624600  | -0.12663300 |
| O       | 2.51768400  | 1.80816900  | 1.37968000  |
| H       | 1.57168500  | 1.79010300  | 1.14660200  |
| H       | 2.92324900  | 1.86854700  | 0.49633600  |
| O       | 2.77492400  | 1.27436500  | -1.51739400 |
| H       | 1.82711500  | 1.46233600  | -1.41017200 |
| H       | 2.84820300  | 0.37038200  | -1.14581200 |
| O       | 2.73108300  | -1.02121400 | 0.19664800  |
| H       | 1.81812100  | -1.37626200 | 0.14161800  |
| H       | 2.67294000  | -0.34707900 | 0.89427700  |

*inv-S<sub>N</sub>2*

## 3RC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.03763400  | 2.10690200  | 0.41913600  |
| H  | 1.24169800  | 1.98045400  | 1.49058400  |
| H  | 0.11246100  | 2.69146400  | 0.30396600  |
| H  | 1.87360300  | 2.65445200  | -0.03793500 |
| C  | 0.79727600  | 0.77336400  | -0.25347000 |
| H  | -0.02913500 | 0.21452200  | 0.20189900  |
| H  | 0.63554400  | 0.86917200  | -1.32995200 |
| Br | 2.41748800  | -0.42769500 | -0.11120300 |
| O  | -2.14731100 | -0.16160500 | 0.78655800  |
| H  | -2.29788500 | -0.13597000 | 1.73854000  |
| O  | -1.37907800 | -2.62976300 | 0.13620000  |
| H  | -0.42870300 | -2.53898300 | 0.00408900  |
| H  | -1.67684500 | -1.70238700 | 0.39941400  |
| O  | -4.49296800 | -0.48694100 | -0.44898500 |
| H  | -4.34269100 | -1.32258100 | -0.90520100 |
| H  | -3.63236700 | -0.35678300 | 0.06012900  |
| O  | -2.21375900 | 2.25212600  | -0.27830400 |
| H  | -3.04611100 | 2.19876100  | -0.76162500 |
| H  | -2.16619500 | 1.34507700  | 0.17045700  |

## 3TS(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.50635200  | 1.75936000  | 0.74044200  |
| H  | 1.10535400  | 1.84442200  | 1.65519700  |
| H  | -0.47806400 | 2.21616700  | 0.90451700  |
| H  | 1.00933700  | 2.31638000  | -0.05760500 |
| C  | 0.33161600  | 0.32089300  | 0.34623600  |
| H  | 0.41371900  | -0.47569000 | 1.06819800  |
| H  | 0.06062000  | 0.06307200  | -0.66631200 |
| Br | 2.71329900  | -0.21392900 | -0.23906900 |
| O  | -1.77756400 | 0.10107900  | 0.67602400  |
| H  | -1.88586200 | 0.24133000  | 1.62571200  |
| O  | -1.68953800 | -2.58778500 | 0.22539300  |
| H  | -0.84373600 | -2.73747800 | -0.21188600 |
| H  | -1.69862400 | -1.61150000 | 0.42200600  |
| O  | -4.22908000 | -0.79115000 | -0.38180500 |
| H  | -3.94082900 | -1.69538500 | -0.56335600 |
| H  | -3.42075800 | -0.40603900 | 0.02820200  |
| O  | -2.83921800 | 2.26399000  | -0.66001500 |
| H  | -3.60918800 | 1.84896200  | -1.06683800 |
| H  | -2.42203700 | 1.51268900  | -0.16727600 |

## 3PC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.94803700 | 3.15595200  | 0.12155800  |
| H  | 0.07192000  | 3.07491200  | 0.52125400  |
| H  | -1.65416800 | 3.17834500  | 0.96432400  |
| H  | -1.03289400 | 4.10492400  | -0.43207200 |
| C  | -1.24749500 | 1.97583700  | -0.79948100 |
| H  | -0.54686100 | 1.97702300  | -1.65115400 |
| H  | -2.26928600 | 2.04934900  | -1.20104300 |
| Br | 2.02676600  | 0.13945800  | 0.16146900  |
| O  | -1.17569600 | 0.72519200  | -0.11784400 |
| H  | -0.22034100 | 0.53484000  | 0.06410800  |
| O  | 0.66535100  | -2.87758000 | -0.13984500 |
| H  | 1.15810900  | -2.02219100 | -0.17084000 |
| H  | 0.50654100  | -2.99054700 | 0.80529400  |
| O  | -1.89006500 | -1.93698500 | -1.09035900 |
| H  | -1.04955500 | -2.37483200 | -0.84700600 |
| H  | -1.67175200 | -0.99239800 | -0.98650800 |
| O  | -3.27346000 | -0.96502900 | 1.29889200  |
| H  | -3.00266300 | -1.55334500 | 0.56991700  |
| H  | -2.66171500 | -0.22262500 | 1.17311200  |

*ret-S<sub>N</sub>2*

## 3RC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.03771100  | 2.10699100  | -0.41870800 |
| H  | 0.11256100  | 2.69156200  | -0.30338600 |
| H  | 1.24169500  | 1.98071000  | -1.49019100 |
| H  | 1.87373600  | 2.65443300  | 0.03839100  |
| C  | 0.79735300  | 0.77334600  | 0.25368800  |
| H  | 0.63575800  | 0.86897200  | 1.33020800  |
| H  | -0.02914500 | 0.21463000  | -0.20168700 |
| Br | 2.41748000  | -0.42778300 | 0.11103600  |
| O  | -2.14718400 | -0.16141800 | -0.78637700 |
| H  | -2.29762100 | -0.13581700 | -1.73838100 |
| O  | -2.21384900 | 2.25243500  | 0.27815700  |
| H  | -2.16623800 | 1.34530400  | -0.17044200 |
| H  | -3.04617700 | 2.19914100  | 0.76152200  |
| O  | -1.37917000 | -2.62961200 | -0.13588100 |
| H  | -1.67682100 | -1.70221200 | -0.39913400 |
| H  | -0.42878600 | -2.53893900 | -0.00376600 |
| O  | -4.49304200 | -0.48731700 | 0.44866400  |
| H  | -3.63235800 | -0.35689400 | -0.06024200 |
| H  | -4.34284500 | -1.32320400 | 0.90445000  |

## 3TS(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.47866900 | -2.43352300 | 0.53843400  |
| H  | -0.32164700 | -3.18105600 | 1.34630700  |
| H  | 0.32048300  | -2.60139500 | -0.19063600 |
| H  | -1.46486400 | -2.59287000 | 0.09256800  |
| C  | -0.36370200 | -1.11886000 | 1.20058700  |
| H  | -1.23250600 | -0.70150500 | 1.69610300  |
| H  | 0.60310300  | -0.80708300 | 1.56961700  |
| Br | -2.05161600 | 0.39203200  | -0.43617600 |
| O  | 1.22939600  | 0.04193700  | -0.21873300 |
| H  | 0.55406000  | 0.19774900  | -0.89277000 |
| O  | 2.71777700  | -2.14483100 | -0.43844500 |
| H  | 2.15572500  | -1.31181400 | -0.40869100 |
| H  | 3.60979100  | -1.80861200 | -0.57675200 |
| O  | 0.82875000  | 2.16797600  | 1.43506400  |
| H  | 1.00685000  | 1.39455600  | 0.83281200  |
| H  | -0.08544400 | 2.38605300  | 1.21339400  |
| O  | 3.45398200  | 1.59693100  | -0.67379000 |
| H  | 2.66764200  | 0.99760800  | -0.59248700 |
| H  | 3.20834000  | 2.32545500  | -0.09020800 |

### 3PC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.07024100 | 1.25693300  | -0.50989700 |
| H  | -3.86760700 | 1.96728200  | -0.23866000 |
| H  | -3.49968600 | 0.47437000  | -1.15136300 |
| H  | -2.30466100 | 1.79615500  | -1.08435300 |
| C  | -2.45570400 | 0.64379700  | 0.74618300  |
| H  | -2.04409100 | 1.43883500  | 1.39104300  |
| H  | -3.22105700 | 0.10423800  | 1.32412000  |
| Br | 1.31653400  | 1.28793000  | -0.30700300 |
| O  | -1.43975800 | -0.30871600 | 0.44478700  |
| H  | -0.65473400 | 0.18182800  | 0.09295800  |
| O  | -1.16293300 | -2.89467500 | -1.04721900 |
| H  | -1.46215400 | -2.07672400 | -0.61753900 |
| H  | -0.19145800 | -2.80723700 | -0.99871900 |
| O  | 0.93303800  | -1.13885700 | 2.08892800  |
| H  | -0.00350600 | -1.09915600 | 1.83189500  |
| H  | 1.28342200  | -0.33407500 | 1.65669300  |
| O  | 1.64798800  | -2.24280700 | -0.54391900 |
| H  | 1.70000200  | -1.31425400 | -0.83585800 |
| H  | 1.51582800  | -2.13274900 | 0.41653000  |

**HO<sup>-</sup>(PCM, H<sub>2</sub>O) + CH<sub>3</sub>CH<sub>2</sub>Br (B3LYP):****R**HO<sup>-</sup>

|   |            |            |             |
|---|------------|------------|-------------|
| O | 0.00000000 | 0.00000000 | 0.10745700  |
| H | 0.00000000 | 0.00000000 | -0.85965500 |

CH<sub>3</sub>CH<sub>2</sub>Br

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.09823100 | -0.40538100 | 0.00000000  |
| H  | -2.01949900 | -1.03780600 | -0.89303500 |
| H  | -3.09267700 | 0.06719700  | 0.00000600  |
| H  | -2.01949200 | -1.03781400 | 0.89302800  |
| C  | -1.05118600 | 0.68902700  | 0.00000000  |
| H  | -1.09107700 | 1.31482800  | -0.89543900 |
| H  | -1.09107700 | 1.31482800  | 0.89543900  |
| Br | 0.80600900  | -0.06637500 | 0.00000000  |

***anti-E2***

RC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.29516400  | -0.39805500 | -0.00109800 |
| C  | 1.07938200  | 0.89710200  | -0.02634300 |
| H  | 0.46527400  | -1.01477700 | -0.88737700 |
| H  | 0.47410400  | -0.98502800 | 0.90351100  |
| H  | 0.86901700  | 1.51231900  | 0.85731600  |
| H  | 2.15264100  | 0.64903200  | -0.02778400 |
| H  | 0.86148200  | 1.48206100  | -0.92866500 |
| O  | 5.15439700  | -0.33282500 | -0.03408400 |
| H  | 4.63510700  | 0.35508000  | 0.40410200  |
| Br | -1.68400200 | -0.06658200 | 0.00332000  |

TS(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.63644900  | -0.48047800 | 0.00282200  |
| C  | 1.49938000  | 0.67440000  | -0.04060400 |
| H  | 0.60336700  | -1.11007000 | -0.88684500 |
| H  | 0.61810200  | -1.05153500 | 0.93154900  |
| H  | 1.43351800  | 1.31980600  | 0.84481600  |
| H  | 2.67340200  | 0.20435500  | -0.02630900 |
| H  | 1.42447500  | 1.25851200  | -0.96659400 |
| O  | 4.02180400  | -0.25689100 | -0.05829800 |
| H  | 4.50319800  | 0.25473800  | 0.60645900  |
| Br | -1.60701300 | 0.00045100  | 0.00542900  |

PC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.54640500  | 0.23374200  | -0.22365300 |
| C  | 4.22261000  | 1.34080200  | 0.10563700  |
| H  | 3.40546200  | -0.06238800 | -1.26458900 |
| H  | 3.10094300  | -0.41175100 | 0.53528900  |
| H  | 4.35561700  | 1.64179200  | 1.14622300  |
| H  | 5.93905000  | -0.48159400 | 0.01319700  |
| H  | 4.65996200  | 1.99135600  | -0.65374000 |
| O  | 6.78007300  | -0.96422100 | -0.02939500 |
| H  | 6.83504400  | -1.42530000 | 0.81756800  |
| Br | -3.69002100 | -0.08530300 | 0.00998000  |

P1(E)

H<sub>2</sub>O

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.00000000 | 0.00000000  | 0.11868500  |
| H | 0.00000000 | 0.76259700  | -0.47474000 |
| H | 0.00000000 | -0.76259700 | -0.47474000 |

CH<sub>2</sub>=CH<sub>2</sub>

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000  | 0.66833900  |
| H | 0.00000000 | 0.92921000  | 1.24125500  |
| H | 0.00000000 | -0.92921000 | 1.24125500  |
| C | 0.00000000 | 0.00000000  | -0.66833900 |
| H | 0.00000000 | -0.92921000 | -1.24125500 |
| H | 0.00000000 | 0.92921000  | -1.24125500 |

*syn-E2*

RC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.60192900 | 1.77802700  | -0.36578500 |
| H  | -0.86609100 | 2.78919700  | -0.01908900 |
| H  | -1.49575800 | 1.14606100  | -0.28888000 |
| H  | -0.30044700 | 1.84448800  | -1.41851200 |
| C  | 0.52434100  | 1.25742800  | 0.50266000  |
| H  | 1.43424100  | 1.85794900  | 0.42342000  |
| H  | 0.23689100  | 1.15024600  | 1.55181500  |
| Br | 1.09276500  | -0.58499900 | -0.04993000 |
| O  | -4.19417800 | -0.71346800 | 0.08479000  |
| H  | -3.23667200 | -0.81795700 | -0.00076800 |

TS(sE)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.81863400 | 1.06505400  | -0.00210200 |
| H | -2.35624400 | 1.37160500  | 0.90547900  |
| H | -1.94620100 | -0.17157400 | -0.00098900 |
| H | -2.35064600 | 1.37131600  | -0.91300900 |
| C | -0.43970300 | 1.51655500  | 0.00237300  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.03117400 | 1.96004800  | -0.90420600 |
| H  | -0.03576700 | 1.95396700  | 0.91394800  |
| Br | 1.10873200  | -0.20872000 | -0.00031600 |
| O  | -2.16199200 | -1.59772200 | 0.00058700  |
| H  | -1.23963200 | -1.88802500 | 0.00349500  |

PC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.66976100  | -0.51553200 | 0.66481600  |
| H  | 3.11927500  | -1.29223800 | 1.19849700  |
| H  | 1.66105200  | 0.95995200  | 0.00994100  |
| H  | 4.20278500  | 0.21583500  | 1.27485400  |
| C  | 3.69642300  | -0.46709700 | -0.67207300 |
| H  | 4.25232100  | 0.30568200  | -1.20589600 |
| H  | 3.16876000  | -1.20233700 | -1.28206200 |
| Br | -1.94913800 | -0.19937500 | -0.00306300 |
| O  | 0.93693400  | 1.60341300  | 0.01792600  |
| H  | 0.12306600  | 1.05970600  | 0.01201900  |

*inv-S<sub>N</sub>2*

RC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.40317400 | 1.88181800  | 0.16793600  |
| H  | -0.37213600 | 1.84118200  | 1.26383800  |
| H  | -1.35997300 | 2.33642600  | -0.13210200 |
| H  | 0.40978300  | 2.52636900  | -0.18872900 |
| C  | -0.32386700 | 0.49780800  | -0.44190100 |
| H  | -1.10926300 | -0.17083400 | -0.08003900 |
| H  | -0.32107100 | 0.51511000  | -1.53483500 |
| Br | 1.38835500  | -0.42686400 | 0.04673100  |
| O  | -4.52964300 | -0.77361000 | 0.11026900  |
| H  | -5.24038400 | -0.19688500 | -0.20208600 |

TS(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.24928100  | 1.39237900  | 0.00006100  |
| H  | 0.84470400  | 1.88556200  | -0.89210200 |
| H  | 2.34180800  | 1.49957600  | -0.00038300 |
| H  | 0.84544400  | 1.88563800  | 0.89252200  |
| C  | 0.94323700  | -0.07616900 | 0.00017900  |
| H  | 1.04160500  | -0.63698200 | -0.91803500 |
| H  | 1.04118000  | -0.63681200 | 0.91861100  |
| Br | -1.38372300 | -0.14318400 | -0.00003000 |
| O  | 3.23853400  | -0.65722400 | -0.00029600 |
| H  | 3.25219900  | -1.62500100 | 0.00136100  |

PC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.70146600 | 1.15669200  | -0.13020800 |
| H  | -3.27168700 | 2.08945700  | 0.26060700  |
| H  | -4.73661400 | 1.07590700  | 0.23019000  |
| H  | -3.71667300 | 1.21661400  | -1.22752900 |
| C  | -2.87476000 | -0.02853400 | 0.33323900  |
| H  | -2.85552500 | -0.07680800 | 1.43430200  |
| H  | -1.83564700 | 0.06428600  | -0.02212500 |
| Br | 2.47320300  | 0.01906100  | -0.01116500 |
| O  | -3.46879700 | -1.22786900 | -0.19850900 |
| H  | -2.93824900 | -1.98260400 | 0.08521900  |

P1(S)  
CH<sub>3</sub>CH<sub>2</sub>OH

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.21708200  | -0.24516500 | 0.02166500  |
| H | 2.08419200  | 0.42514200  | -0.07122500 |
| H | 1.26851800  | -0.97859900 | -0.79684100 |
| H | 1.29344400  | -0.78216400 | 0.97742900  |
| C | -0.07411000 | 0.55913900  | -0.04725700 |
| H | -0.12964300 | 1.11681600  | -0.99666100 |
| H | -0.12023800 | 1.28787900  | 0.77266300  |
| O | -1.24789900 | -0.25713500 | 0.11031200  |
| H | -1.27091400 | -0.89583400 | -0.61431400 |

*ret-S<sub>N</sub>2*

RC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.49823700  | 2.01003300  | -0.23626300 |
| H  | 0.60790900  | 1.85104800  | -1.31673100 |
| H  | 1.36626700  | 2.59251200  | 0.11125100  |
| H  | -0.40623200 | 2.60445200  | -0.05410000 |
| C  | 0.48063900  | 0.69704400  | 0.51891100  |
| H  | 1.36013500  | 0.07041400  | 0.31835400  |
| H  | 0.32895300  | 0.83417800  | 1.59330200  |
| Br | -1.08694700 | -0.43924500 | -0.04390300 |
| O  | 3.13236000  | -0.91619800 | -0.05817900 |
| H  | 3.85398800  | -1.49192100 | -0.34591200 |

TS(rS)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.95171700 | -1.31425900 | -0.39835600 |
| H | -2.30232400 | -0.75648200 | -1.27327400 |
| H | -2.84361600 | -1.83983500 | 0.01188900  |
| H | -1.21151000 | -2.07113000 | -0.67336100 |
| C | -1.53405200 | -0.43654300 | 0.69795900  |
| H | -2.07303600 | 0.48932800  | 0.88120800  |
| H | -0.85978600 | -0.81373200 | 1.46063300  |

|                                   |             |             |             |
|-----------------------------------|-------------|-------------|-------------|
| Br                                | 1.22837400  | -0.06961200 | -0.02064300 |
| O                                 | -1.52681800 | 2.00596900  | -0.15287700 |
| H                                 | -0.57364900 | 1.88531600  | -0.25920200 |
| PC(rS)                            |             |             |             |
| C                                 | 2.75311300  | 1.00622600  | -0.16528700 |
| H                                 | 3.15826500  | 0.90686100  | -1.18237400 |
| H                                 | 3.49811700  | 1.52649900  | 0.45538100  |
| H                                 | 1.84978200  | 1.63134900  | -0.21003200 |
| C                                 | 2.43951400  | -0.36401500 | 0.42661200  |
| H                                 | 3.35250000  | -0.97406600 | 0.47478900  |
| H                                 | 2.05996800  | -0.25494100 | 1.45663600  |
| Br                                | -1.65060000 | 0.08374400  | 0.01758000  |
| O                                 | 1.50937000  | -1.11324800 | -0.36407700 |
| H                                 | 0.62164500  | -0.71403700 | -0.26502500 |
| <b><i>PT</i></b>                  |             |             |             |
| P1(PT)                            |             |             |             |
| CH <sub>3</sub> CHBr <sup>-</sup> |             |             |             |
| C                                 | 2.14259900  | -0.37971000 | 0.02204700  |
| H                                 | 2.13522700  | -1.08819800 | -0.82160100 |
| H                                 | 3.16122400  | 0.05331100  | 0.05949300  |
| H                                 | 2.00946200  | -0.96488700 | 0.95422200  |
| C                                 | 1.20987900  | 0.80363200  | -0.19806800 |
| H                                 | 1.16684500  | 1.35982700  | 0.76066300  |
| Br                                | -0.81678900 | -0.05438800 | 0.00295300  |
| <b><i>Dits</i></b>                |             |             |             |
| TS(Dits)                          |             |             |             |
| C                                 | 1.12805100  | 1.74105600  | -0.27755300 |
| H                                 | 1.52317300  | 1.31210400  | -1.22914100 |
| H                                 | 0.49681700  | 2.60360100  | -0.58113400 |
| H                                 | 1.99917500  | 2.17185100  | 0.24725200  |
| C                                 | 0.47646700  | 0.77578800  | 0.65811500  |
| H                                 | 0.83872200  | 0.38709600  | 1.60200700  |
| H                                 | 1.73653500  | -0.63861400 | 0.21803300  |
| Br                                | -1.07214500 | -0.23636300 | -0.04742500 |
| O                                 | 2.41999900  | -1.33989200 | -0.03327700 |
| H                                 | 1.94356200  | -1.94526100 | -0.61428200 |

**HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>) + CH<sub>3</sub>CH<sub>2</sub>Br (MP2):**

**1R**HO<sup>-</sup>(H<sub>2</sub>O<sub>w</sub>)

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.25585200 | 0.08659800  | -0.07417600 |
| H | -1.59198200 | -0.53918100 | 0.58507500  |
| O | 1.25097800  | -0.09815100 | -0.05013800 |
| H | 1.46955400  | 0.68188300  | 0.47539500  |
| H | 0.16141900  | -0.05028400 | -0.06595500 |

CH<sub>3</sub>CH<sub>2</sub>Br

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.07597900 | -0.40288300 | -0.00000400 |
| H  | -1.98325600 | -1.03768400 | -0.89320200 |
| H  | -3.07803800 | 0.05833300  | 0.00093500  |
| H  | -1.98183100 | -1.03909600 | 0.89213400  |
| C  | -1.01939700 | 0.69212600  | 0.00006500  |
| H  | -1.07574300 | 1.32389700  | -0.89603500 |
| H  | -1.07525500 | 1.32333800  | 0.89625200  |
| Br | 0.79332500  | -0.06755000 | -0.00001300 |

***anti-E2***

1RC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.41642400  | 1.45453600  | 0.80180100  |
| H  | -0.16844700 | 2.33731900  | 0.49681700  |
| H  | 1.49534100  | 1.66044600  | 0.69023200  |
| H  | 0.17479000  | 1.21105900  | 1.84850900  |
| C  | 0.15158200  | 0.27407000  | -0.11009000 |
| H  | 0.39186300  | 0.49917400  | -1.15397200 |
| H  | 0.69605500  | -0.62228600 | 0.20814400  |
| Br | -1.78450800 | -0.23117700 | -0.10022600 |
| O  | 2.93828200  | 0.72360200  | -0.75698900 |
| H  | 3.84646700  | 0.90083600  | -1.04224100 |
| O  | 2.90335300  | -1.43058600 | 0.56199600  |
| H  | 2.96910700  | -0.51508500 | 0.00805300  |
| H  | 2.91149700  | -2.09602600 | -0.13795800 |

1TS(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.60445100  | 0.50001000  | 0.72808100  |
| H  | 0.36397500  | 1.48053900  | 1.16769500  |
| H  | 1.82619400  | 0.61737900  | 0.15976800  |
| H  | 0.69063700  | -0.27786500 | 1.50116100  |
| C  | -0.22957800 | 0.13452000  | -0.39856700 |
| H  | -0.33817800 | 0.90156300  | -1.17413500 |
| H  | -0.02967900 | -0.85253600 | -0.83138900 |
| Br | -2.36897400 | -0.15917000 | -0.00792900 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 3.00890000 | 0.71563200  | -0.36805500 |
| H | 3.21751900 | 1.66175400  | -0.36386800 |
| O | 5.16291100 | -0.75619600 | 0.17592800  |
| H | 4.35039800 | -0.18045800 | 0.02216800  |
| H | 5.20950700 | -1.26207500 | -0.64397600 |

1PC(aE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.06694500  | -1.60567700 | -0.03667000 |
| H  | 0.97493700  | -1.50840500 | -0.07132200 |
| H  | 1.48519000  | 0.42512900  | 1.51686800  |
| H  | 2.49495300  | -2.51711100 | 0.39545800  |
| C  | 2.86568000  | -0.62155900 | -0.51055900 |
| H  | 2.43261500  | 0.28851500  | -0.93854100 |
| H  | 3.95721400  | -0.70939200 | -0.47564900 |
| Br | -1.54485500 | -0.35064700 | -0.08665100 |
| O  | 0.82073400  | 1.08524000  | 1.76530400  |
| H  | 0.00508800  | 0.68899300  | 1.37712600  |
| O  | 0.71266900  | 2.09508600  | -1.05158800 |
| H  | 0.87720600  | 2.07576900  | -0.09243200 |
| H  | -0.02024300 | 1.44994000  | -1.10508700 |

1P1(E)

H<sub>2</sub>O

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.00000000 | 0.00000000  | 0.11910300  |
| H | 0.00000000 | 0.76051500  | -0.47641100 |
| H | 0.00000000 | -0.76051500 | -0.47641100 |

CH<sub>2</sub>=CH<sub>2</sub>

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 0.00000000  | 0.67466200  | 0.00000000 |
| H | 0.93365900  | 1.24294700  | 0.00000000 |
| H | -0.93365200 | 1.24297000  | 0.00000000 |
| C | 0.00000000  | -0.67466200 | 0.00000000 |
| H | -0.93365900 | -1.24294700 | 0.00000000 |
| H | 0.93365200  | -1.24297000 | 0.00000000 |

*syn-E2*

1RC(sE)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.50586200  | -1.23672300 | 0.93384800  |
| H | 1.58283900  | -1.43663600 | 0.79742400  |
| H | -0.06400100 | -2.17322300 | 0.82070100  |
| H | 0.31273400  | -0.82258000 | 1.93619000  |
| C | 0.14377000  | -0.23803800 | -0.14657900 |
| H | 0.65931800  | 0.71934200  | -0.01150000 |
| H | 0.33738100  | -0.62848900 | -1.15039100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Br | -1.81294300 | 0.18823200  | -0.10735800 |
| O  | 2.98231600  | -0.79690500 | -0.72218700 |
| H  | 3.73799300  | -0.81126900 | -1.32758600 |
| O  | 2.85487200  | 1.48765800  | 0.34036000  |
| H  | 2.94608900  | 0.53070000  | -0.13795300 |
| H  | 3.34535100  | 1.35657400  | 1.16165800  |

#### 1TS(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.33522000  | 1.83080400  | 0.15959200  |
| H  | 0.90935700  | 2.32660500  | -0.63826500 |
| H  | 1.10237200  | 0.77543900  | 0.41736600  |
| H  | 0.34271700  | 2.41292200  | 1.09373500  |
| C  | -1.02010100 | 1.46976900  | -0.27789700 |
| H  | -1.86477800 | 1.86945600  | 0.29649000  |
| H  | -1.21394100 | 1.54074800  | -1.35505900 |
| Br | -1.52785000 | -0.60006300 | -0.03446500 |
| O  | 1.88333000  | -0.23809100 | 0.67513700  |
| H  | 1.27895100  | -0.98865100 | 0.56684400  |
| O  | 4.23470600  | -0.48912100 | -0.50528300 |
| H  | 3.30365500  | -0.40968700 | -0.11295600 |
| H  | 4.78141300  | -0.51036300 | 0.28912600  |

#### 1PC(sE)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.86575900 | -0.62146700 | -0.51056100 |
| H  | -2.43273900 | 0.28868400  | -0.93842600 |
| H  | -1.48532400 | 0.42505500  | 1.51668400  |
| H  | -3.95729200 | -0.70929300 | -0.47562400 |
| C  | -2.06697000 | -1.60558900 | -0.03676700 |
| H  | -2.49487400 | -2.51706200 | 0.39525100  |
| H  | -0.97496400 | -1.50821300 | -0.07147100 |
| Br | 1.54490000  | -0.35060600 | -0.08664300 |
| O  | -0.82082600 | 1.08502200  | 1.76535200  |
| H  | -0.00524900 | 0.68894600  | 1.37705900  |
| O  | -0.71265300 | 2.09495300  | -1.05155400 |
| H  | -0.87719200 | 2.07576900  | -0.09241000 |
| H  | 0.02032500  | 1.44986900  | -1.10497500 |

#### *inv-S<sub>N</sub>2*

##### 1RC(iS)

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.58683800 | -1.30358200 | 0.40259000  |
| H | 0.47306200 | -1.13293500 | 1.48387100  |
| H | 1.66509300 | -1.35526400 | 0.17189000  |
| H | 0.09425800 | -2.25301900 | 0.13435500  |
| C | 0.02602300 | -0.13093400 | -0.37865200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.54448800  | 0.80341600  | -0.10587300 |
| H  | 0.07367100  | -0.29253400 | -1.46377200 |
| Br | -1.92054100 | 0.11456600  | -0.01184200 |
| O  | 2.41034100  | 1.42184700  | 0.28640500  |
| H  | 2.89951100  | 2.24733400  | 0.15824000  |
| O  | 3.86065500  | -0.55055100 | -0.34623700 |
| H  | 4.34596800  | -0.70243600 | 0.47465300  |
| H  | 3.27775800  | 0.31236500  | -0.10387300 |

#### 1TS(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.64126700  | -1.09522500 | 0.61146500  |
| H  | 0.10860000  | -1.37880600 | 1.53104000  |
| H  | 1.72637500  | -1.12635200 | 0.78192000  |
| H  | 0.37273100  | -1.81367600 | -0.17619400 |
| C  | 0.25884700  | 0.30521000  | 0.19562900  |
| H  | 0.09093500  | 1.06647100  | 0.94639800  |
| H  | 0.42396800  | 0.62475800  | -0.82607500 |
| Br | -2.02126500 | 0.02588700  | -0.15153800 |
| O  | 2.29695200  | 0.99404000  | 0.45413000  |
| H  | 2.33199400  | 1.92261900  | 0.17468200  |
| O  | 4.20512400  | -0.39081800 | -0.67431600 |
| H  | 4.81906100  | -0.46283400 | 0.06658900  |
| H  | 3.45331100  | 0.17607800  | -0.27560500 |

#### 1PC(iS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.15988900  | -0.99467800 | 0.43850900  |
| H  | 1.60769500  | -1.15496300 | 1.43299800  |
| H  | 1.78283700  | -1.49386100 | -0.32216700 |
| H  | 0.14718600  | -1.42459900 | 0.41705200  |
| C  | 1.03150200  | 0.48668800  | 0.14464100  |
| H  | 0.35520700  | 0.96526500  | 0.86704300  |
| H  | 0.61280500  | 0.64696100  | -0.85972900 |
| Br | -2.42085200 | -0.02743400 | -0.08952100 |
| O  | 2.36835500  | 1.08471700  | 0.23875000  |
| H  | 2.28300100  | 2.01461000  | -0.00804100 |
| O  | 4.69240600  | -0.38440700 | -0.42113500 |
| H  | 4.41841400  | -1.28620000 | -0.21427500 |
| H  | 3.88824200  | 0.13842500  | -0.21946600 |

#### 1P1(S)

CH<sub>3</sub>CH<sub>2</sub>OH

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.21675300 | -0.24450000 | 0.02229700  |
| H | 2.09016800 | 0.42348600  | -0.05359700 |
| H | 1.27271400 | -0.96954700 | -0.80679200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.27352300  | -0.79642800 | 0.97244200  |
| C | -0.07613200 | 0.56147600  | -0.04751200 |
| H | -0.12781800 | 1.12975500  | -0.99414600 |
| H | -0.12678200 | 1.28407500  | 0.78005700  |
| O | -1.24663600 | -0.25899300 | 0.10850800  |
| H | -1.25244100 | -0.90125400 | -0.61473800 |

*ret-S<sub>N</sub>2*

1RC(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.41662000 | 1.45358900  | 0.80299000  |
| H  | -0.17491800 | 1.20907400  | 1.84946700  |
| H  | -1.49558900 | 1.65939800  | 0.69166400  |
| H  | 0.16806300  | 2.33685400  | 0.49888100  |
| C  | -0.15153800 | 0.27409100  | -0.11012800 |
| H  | -0.69603700 | -0.62260900 | 0.20712100  |
| H  | -0.39164000 | 0.50025300  | -1.15381900 |
| Br | 1.78454300  | -0.23111300 | -0.10033800 |
| O  | -2.90385100 | -1.42983800 | 0.56240300  |
| H  | -2.91306900 | -2.09538900 | -0.13736000 |
| O  | -2.93762800 | 0.72339700  | -0.75822100 |
| H  | -2.96913800 | -0.51458900 | 0.00801900  |
| H  | -3.84589300 | 0.90139900  | -1.04275200 |

1TS(rS)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.91273600 | 1.94602300  | 0.29556500  |
| H  | -1.87634500 | 1.71093500  | 0.76159600  |
| H  | -0.97748700 | 2.89305000  | -0.28099900 |
| H  | -0.16601600 | 2.09331800  | 1.09070700  |
| C  | -0.47010900 | 0.84733500  | -0.63074700 |
| H  | -1.25094200 | 0.28621600  | -1.14605100 |
| H  | 0.28581900  | 1.20238900  | -1.34020000 |
| Br | 1.63145500  | -0.30126500 | -0.03888000 |
| O  | -1.24258200 | -0.52719700 | 0.84150900  |
| H  | -0.55754800 | -1.21295300 | 0.81338100  |
| O  | -3.45504100 | -0.92109800 | -0.44625600 |
| H  | -2.56989700 | -0.85249900 | 0.07044500  |
| H  | -4.11045500 | -0.74995600 | 0.24098300  |

1PC(rS)

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.19963100 | -0.49450000 | 1.10042100  |
| H | 2.77882100 | 0.44254000  | 1.12017500  |
| H | 2.71525300 | -1.24450100 | 1.72695800  |
| H | 1.20153400 | -0.29957800 | 1.52051100  |
| C | 2.06043500 | -1.00809000 | -0.33250500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.05371100  | -1.20829400 | -0.77119700 |
| H  | 1.48857900  | -1.95422900 | -0.33392700 |
| Br | -1.54908900 | -0.28546700 | 0.05733600  |
| O  | 1.42392900  | -0.05661800 | -1.19349500 |
| H  | 0.46078000  | -0.10878800 | -0.96492900 |
| O  | 0.58268400  | 2.50166700  | 0.09592600  |
| H  | 1.12505600  | 1.85224200  | -0.38412500 |
| H  | -0.21891600 | 1.96709600  | 0.25284300  |

***PT***

1RC(PT)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.41708600  | 1.45211200  | 0.80414000  |
| H  | -0.16725000 | 2.33579100  | 0.50058600  |
| H  | 1.49610600  | 1.65761300  | 0.69281200  |
| H  | 0.17535400  | 1.20705500  | 1.85047300  |
| C  | 0.15147300  | 0.27332500  | -0.10971900 |
| H  | 0.39187600  | 0.50001100  | -1.15322300 |
| H  | 0.69543700  | -0.62384400 | 0.20709700  |
| Br | -1.78488200 | -0.23086900 | -0.10047100 |
| O  | 2.93715500  | 0.72356200  | -0.75943200 |
| H  | 3.84564200  | 0.90250000  | -1.04267300 |
| O  | 2.90516500  | -1.42889800 | 0.56248400  |
| H  | 2.91439500  | -2.09478600 | -0.13705900 |
| H  | 2.96941000  | -0.51386600 | 0.00752300  |

1TS(PT)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.32322000 | 2.18807900  | 0.57076400  |
| H  | -0.31717500 | 2.55074400  | -0.47203900 |
| H  | 0.36010300  | 2.84366000  | 1.14656400  |
| H  | -1.34923400 | 2.33267800  | 0.97283800  |
| C  | 0.23518000  | 0.76452000  | 0.66016500  |
| H  | 1.69375700  | 0.82570300  | -0.26858700 |
| H  | 0.11694100  | 0.41974400  | 1.70928000  |
| Br | -1.15065500 | -0.43919300 | -0.25599900 |
| O  | 2.55793400  | 0.93692000  | -0.84770200 |
| H  | 2.51582100  | 0.16775800  | -1.43229000 |
| O  | 1.81821800  | -1.98480200 | 0.69827000  |
| H  | 0.89041500  | -2.09060900 | 0.43587800  |
| H  | 1.88131500  | -1.01047200 | 0.67819300  |

1PC(PT)

|   |            |            |             |
|---|------------|------------|-------------|
| C | 0.19103000 | 2.07106200 | 0.43641600  |
| H | 0.38504900 | 2.28706900 | -0.62908600 |
| H | 0.99329200 | 2.56518300 | 1.01958600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.77211300 | 2.55485200  | 0.70637200  |
| C  | 0.27409700  | 0.56553500  | 0.72352600  |
| H  | 1.94715900  | 0.54564900  | -0.29739000 |
| H  | -0.02705200 | 0.41537400  | 1.78245500  |
| Br | -1.33687900 | -0.27224100 | -0.22037300 |
| O  | 2.79825300  | 0.57137000  | -0.82074100 |
| H  | 3.05766500  | -0.35844000 | -0.74453300 |
| O  | 1.71294000  | -1.93271200 | 0.59018700  |
| H  | 1.01504300  | -2.40522800 | 0.11660900  |
| H  | 1.31141100  | -1.00487000 | 0.64381300  |

1P1(PT)

CH<sub>3</sub>CHBr<sup>-</sup>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.07549600  | -0.36492300 | 0.02184600  |
| H  | 2.05892300  | -1.06978800 | -0.82986600 |
| H  | 3.09530600  | 0.07265900  | 0.05863700  |
| H  | 1.93762000  | -0.97265400 | 0.94941500  |
| C  | 1.09888100  | 0.80214300  | -0.19866200 |
| H  | 1.10139100  | 1.38819400  | 0.75136100  |
| Br | -0.77827200 | -0.05833500 | 0.00375300  |

***Dits***

1TS(Dits)

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.57647000  | 1.71259200  | 0.01683900  |
| H  | 1.16332200  | 1.19022100  | -0.78485400 |
| H  | 0.06732900  | 2.55806900  | -0.49800000 |
| H  | 1.31307000  | 2.16576300  | 0.70952300  |
| C  | -0.33657700 | 0.84328700  | 0.82358400  |
| H  | -0.17495500 | 0.48854300  | 1.83960100  |
| H  | 0.92114700  | -0.57981200 | 0.72586600  |
| Br | -1.59507600 | -0.22972400 | -0.19704400 |
| O  | 1.57414500  | -1.34102900 | 0.54008800  |
| H  | 1.08379100  | -1.85074800 | -0.11917400 |
| O  | 3.86034700  | -0.08810600 | -0.44428000 |
| H  | 3.45271500  | 0.75076600  | -0.69611400 |
| H  | 3.08592100  | -0.58465100 | -0.08930100 |