**Table 5a**: Variation in Bond lengths of reactant complexes (R1- R4) of reaction with OH radicals

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RC1 | Bond length (Å) | RC2 | | Bond length  (Å) | RC3 | Bond length  (Å) | RC4 | Bond length (Å) |
| C1,H1 | 1.102 | C1,H1 | 1.103 | | C1,H1 | 1.102 | C1,H1 | 1.101 |
| C1,H2 | 1.098 | C1,H2 | 1.102 | | C1,H2 | 1.104 | C1,H2 | 1.102 |
| C1,H4 | 1.099 | C1,H4 | 1.122 | | C1,H4 | 1.100 | C1,H4 | 1.107 |
| C1,C2 | 1.518 | C1,C2 | 1.512 | | C1,C2 | 1.518 | C1,C2 | 1.517 |
| C2,O2 | 1.416 | C2,O2 | 1.466 | | C2,O2 | 1.422 | C2,O2 | 1.420 |
| C2,C3 | 1.522 | C2,C3 | 1.471 | | C2,C3 | 1.523 | C2,C3 | 1.508 |
| C4,O1 | 1.423 | C4,O1 | 1.392 | | C4,O1 | 1.424 | C4,O1 | 1.415 |
| C4,H9 | 1.108 | C4,H9 | 1.107 | | C4,H9 | 1.105 | C4,H9 | 1.103 |
| O2,H10 | 0.966 | O2,H10 | 0.967 | | O2,H10 | 0.966 | O2,H10 | 0.958 |
| C3,F1 | 1.415 | C3,F1 | 1.450 | | C3,F1 | 1.419 | C3,F1 | 1.373 |

**Table 5b**: Variation in C3, F1 Bond lengths of transition states, Product complexes and Products of reaction with OH radicals

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Transition states | Bond length (Å) | Product complexes | Bond length  (Å) | Products | Bond length  (Å) |
| TS1 | 1.376 | PC1 | 1.474 | P1 | 1.313 |
| 2 | 1.400 | PC2 | 1.543 | P2 | 1.355 |
| TS3 | 1.500 | PC3 | 1.398 | P3 | 1.380 |
| TS4 | 1.456 | PC4 | 1.396 | P4 | 1.566 |

**Table 6a**: Variation in Bond lengths of reactant complexes (R5- R8) of reaction with ClO radicals

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RC5 | Bond length (Å) | RC6 | | Bond length  (Å) | RC7 | Bond length  (Å) | RC8 | Bond length (Å) |
| C1,H1 | 1.099 | C1,H1 | 1.100 | | C1,H1 | 1.099 | C1,H1 | 1.098 |
| C1,H2 | 1.100 | C1,H2 | 1.107 | | C1,H2 | 1.100 | C1,H2 | 1.100 |
| C1,H4 | 1.098 | C1,H4 | 1.101 | | C1,H4 | 1.099 | C1,H4 | 1.102 |
| C1,C2 | 1.514 | C1,C2 | 1.517 | | C1,C2 | 1.516 | C1,C2 | 1.517 |
| C2,O2 | 1.424 | C2,O2 | 1.438 | | C2,O2 | 1.425 | C2,O2 | 1.424 |
| C2,C3 | 1.510 | C2,C3 | 1.507 | | C2,C3 | 1.509 | C2,C3 | 1.510 |
| C4,O1 | 1.414 | C4,O1 | 1.402 | | C4,O1 | 1.412 | C4,O1 | 1.419 |
| C4,H9 | 1.099 | C4,H9 | 1.103 | | C4,H9 | 1.097 | C4,H9 | 1.105 |
| O2,Cl11 | 1.712 | O2,Cl11 | 1.714 | | O2,Cl11 | 1.713 | O2,Cl11 | 1.713 |
| C3,F1 | 1.410 | C3,F1 | 1.414 | | C3,F1 | 1.409 | C3,F1 | 1.399 |

**Table 6b**: Variation in C3, F1 Bond lengths of transition states, Product complexes and Products of reaction with ClO radicals

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Transition states | Bond length (Å) | Product complexes | Bond length  (Å) | Products | Bond length  (Å) |
| TS5 | 1.450 | PC5 | 1.403 | P5 | 1.315 |
| 6 | 1.402 | PC6 | 1.415 | P6 | 1.355 |
| TS7 | 1.403 | PC7 | 1.418 | P7 | 1.382 |
| TS8 | 1.416 | PC8 | 1.394 | P8 | 1.568 |

**Table 7a**: Variation in Bond angles of reactant complexes (R1- R4) of reaction with OH radicals

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RC1 | Bond angle () | RC2 | | Bond angle  () | RC3 | Bond angle  () | RC4 | Bond angle  () |
| <C3F1H7 | 31.44 | <C3F1H7 | 32.58 | | <C3F1H7 | 31.38 | <C3F1H7 | 31.32 |
| <C3H8H7 | 33.75 | <C3H8H7 | 34.98 | | <C3H8H7 | 33.78 | <C3H8H7 | 35.52 |
| <C3C2C1 | 112.75 | <C3C2C1 | 110.10 | | <C3C2C1 | 111.25 | <C3C2C1 | 111.93 |
| <C2O1C3 | 36.84 | <C2O1C3 | 36.12 | | <C2O1C3 | 36.26 | <C2O1C3 | 37.39 |
| <C2O1C4 | 113.88 | <C2O1C4 | 112.62 | | <C2O1C4 | 115.89 | <C2O1C4 | 114.40 |
| <C2O1C1 | 37.99 | <C2O1C1 | 37.66 | | <C2O1C1 | 34.32 | <C2O1C1 | 38.36 |
| <O1C4H5 | 106.18 | <O1C4H5 | 111.86 | | <O1C4H5 | 113.40 | <O1C4H5 | 106.85 |
| <O1C2F1 | 143.00 | <O1C2F1 | 101.46 | | <O1C2F1 | 141.25 | <O1C2F1 | 138.45 |
| <C1C2F1 | 91.33 | <C1C2F1 | 140.35 | | <C1C2F1 | 98.79 | <C1C2F1 | 129.70 |
| < C3C2F1 | 34.32 | < C3C2F1 | 33.02 | | < C3C2F1 | 34.59 | < C3C2F1 | 93.68 |
| <H4H1H2 | 60.30 | <H4H1H2 | 60.63 | | <H4H1H2 | 60.10 | <H4H1H2 | 60.10 |
| <F1H7H8 | 64.34 | <F1H7H8 | 32.62 | | <F1H7H8 | 64.45 | <F1H7H8 | 63.65 |
| <C2H6O1 | 40.11 | <C2H6O1 | 15.12 | | <C2H6O1 | 43.73 | <C2H6O1 | 40.18 |
| <F1O2H10 | 111.98 | <F1O2H10 | 118.23 | | <F1O2H10 | 134.80 | <F1O2H10 | 112.50 |

**Table 7b**:Variation in <C3F1H7 Bond angles of transition states, Product complexes and Products of reaction with OH radicals

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Transition states | Bond angle () | Product complexes | Bond angles  () | Products | Bond angles  () |
| TS1 | 29.14 | PC1 | 39.20 | P1 | 29.49 |
| 2 | 31.13 | PC2 | 31.80 | P2 | 30.88 |
| TS3 | 33.20 | PC3 | 31.14 | P3 | 30.73 |
| TS4 | 31.76 | PC4 | 31.50 | P4 | 29.87 |

**Table 8a**:Variation in Bond angles of reactant complexes (R5- R8) of reaction with ClO radicals

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RC5 | Bond angle () | RC6 | | Bond angle  () | RC7 | Bond angle  () | RC8 | Bond angle  () |
| <C3F1H7 | 30.99 | <C3F1H7 | 30.85 | | <C3F1H7 | 31.08 | <C3F1H7 | 31.79 |
| <C3H8H7 | 36.19 | <C3H8H7 | 33.97 | | <C3H8H7 | 36.00 | <C3H8H7 | 35.42 |
| <C3C2C1 | 112.34 | <C3C2C1 | 112.06 | | <C3C2C1 | 112.48 | <C3C2C1 | 113.34 |
| <C2O1C3 | 34.62 | <C2O1C3 | 34.34 | | <C2O1C3 | 35.32 | <C2O1C3 | 35.05 |
| <C2O1C4 | 113.73 | <C2O1C4 | 116.63 | | <C2O1C4 | 113.05 | <C2O1C4 | 115.84 |
| <C2O1C1 | 37.97 | <C2O1C1 | 33.67 | | <C2O1C1 | 37.72 | <C2O1C1 | 34.25 |
| <O1C4H5 | 111.43 | <O1C4H5 | 112.70 | | <O1C4H5 | 112.64 | <O1C4H5 | 110.19 |
| <O1C2F1 | 97.36 | <O1C2F1 | 99.65 | | <O1C2F1 | 97.88 | <O1C2F1 | 105.15 |
| <C1C2F1 | 91.35 | <C1C2F1 | 93.77 | | <C1C2F1 | 89.82 | <C1C2F1 | 91.89 |
| < C3C2F1 | 33.10 | < C3C2F1 | 32.99 | | < C3C2F1 | 33.15 | < C3C2F1 | 31.29 |
| <H4H1H2 | 60.02 | <H4H1H2 | 60.65 | | <H4H1H2 | 60.12 | <H4H1H2 | 60.99 |
| <F1H7H8 | 64.53 | <F1H7H8 | 62.37 | | <F1H7H8 | 64.42 | <F1H7H8 | 63.65 |
| <C2H6O1 | 40.52 | <C2H6O1 | 44.17 | | <C2H6O1 | 40.45 | <C2H6O1 | 44.04 |
| <F1O2Cl11 | 96.48 | <F1O2H10 | 113.23 | | <F1O2H10 | 95.90 | <F1O2H10 | 139.54 |

**Table 8b**: Variation in <C3F1H7 Bond angles of transition states, Product complexes and Products of reaction with ClO radicals

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Transition states | Bond angle () | Product complexes | Bond angles  () | Products | Bond angles  () |
| TS5 | 31.78 | PC5 | 32.00 | P5 | 28.52 |
| 6 | 31.50 | PC6 | 30.79 | P6 | 32.50 |
| TS7 | 31.73 | PC7 | 30.26 | P7 | 30.28 |
| TS8 | 30.40 | PC8 | 31.40 | P8 | 29.09 |