Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# The Electrophilic Aromatic Bromination of Benzenes: Mechanistic and Regioselective Insights from Density Functional Theory

## Supporting Information

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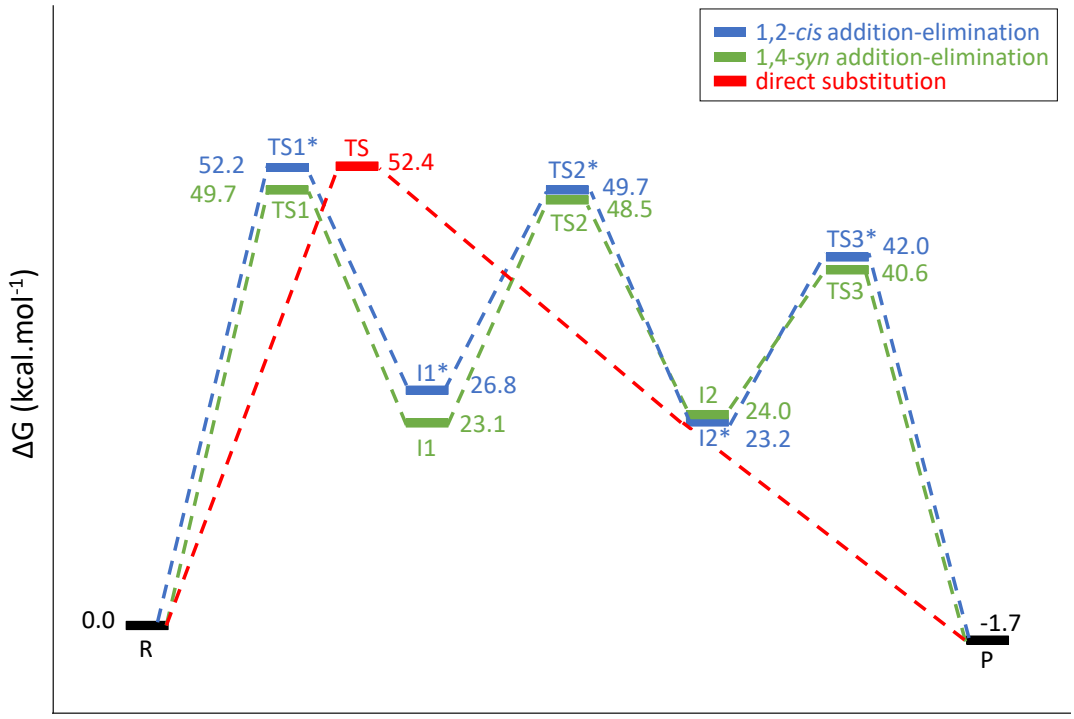


**Figure S1.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of benzene in the apolar $CCl_4$ solvent following a direct substitution (red), 1,2-*cis* (blue) or 1,4-*syn* (green) addition elimination pathway. The reactants (R) correspond to benzene, HBr and $Br_2$, while bromobenzene and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

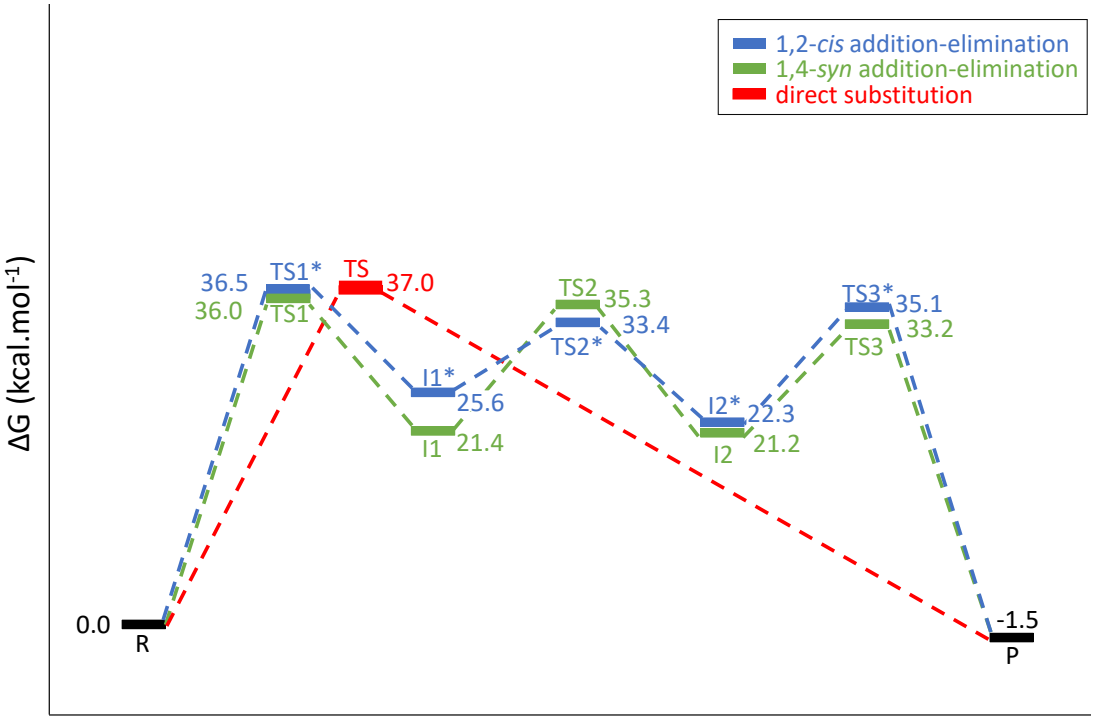


**Figure S2.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of benzene in the polar acetonitrile solvent following a direct substitution (red), 1,2-*cis* (blue) or 1,4-*syn* (green) addition elimination pathway. The reactants (R) correspond to benzene, HBr and $Br_2$, while bromobenzene and 2 HBr molecules are

obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

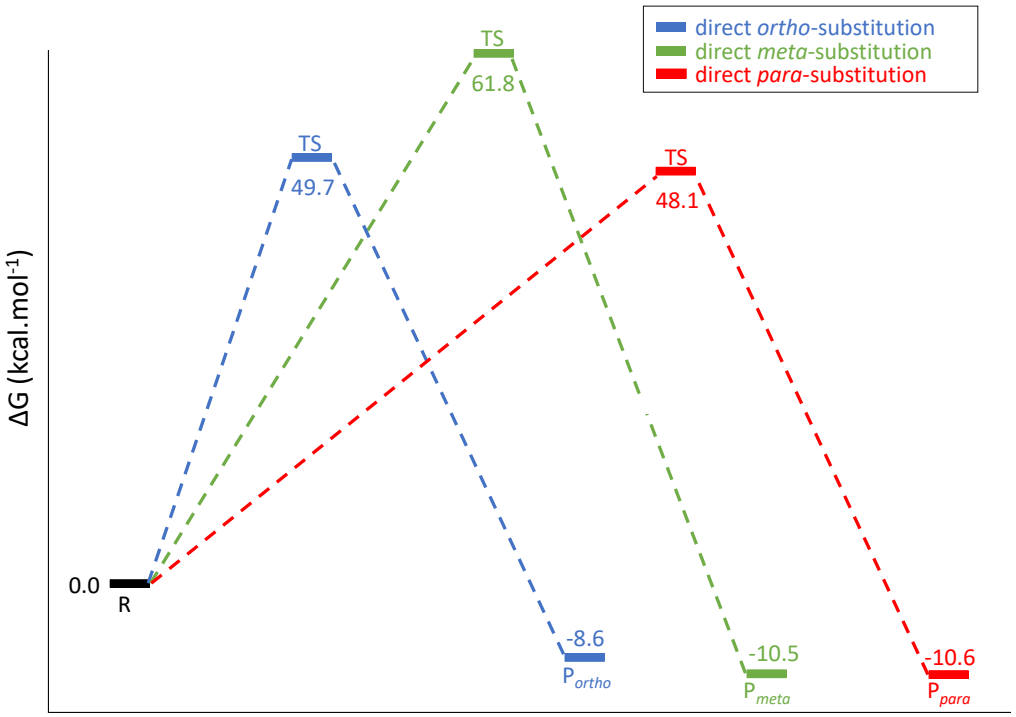


**Figure S3.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of anisole in the gas phase following a direct concerted substitution pathway at the *ortho* (blue), *meta* (green) or *para* (red) position. The reactants (R) correspond to anisole, HBr and $Br_2$, while bromoanisole and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

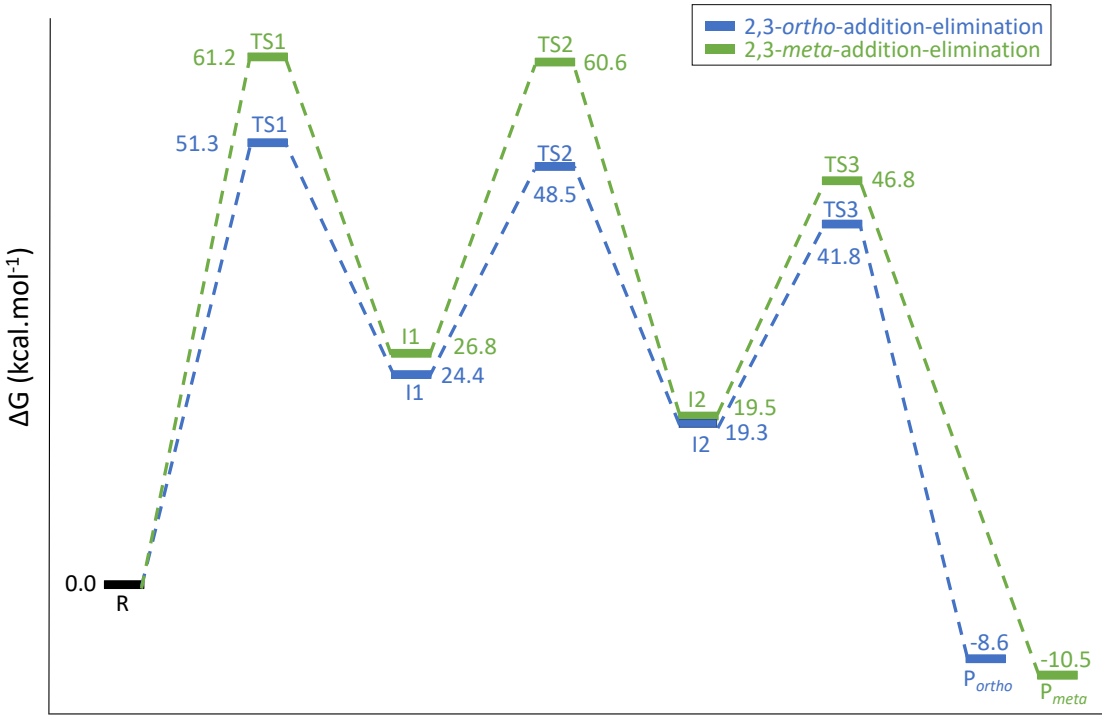


**Figure S4.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of anisole in the gas phase following a 2,3-addition-elimination pathway at the *ortho* (blue) or *meta* (green) position. The reactants (R) correspond to anisole, HBr and $Br_2$, while bromoanisole and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

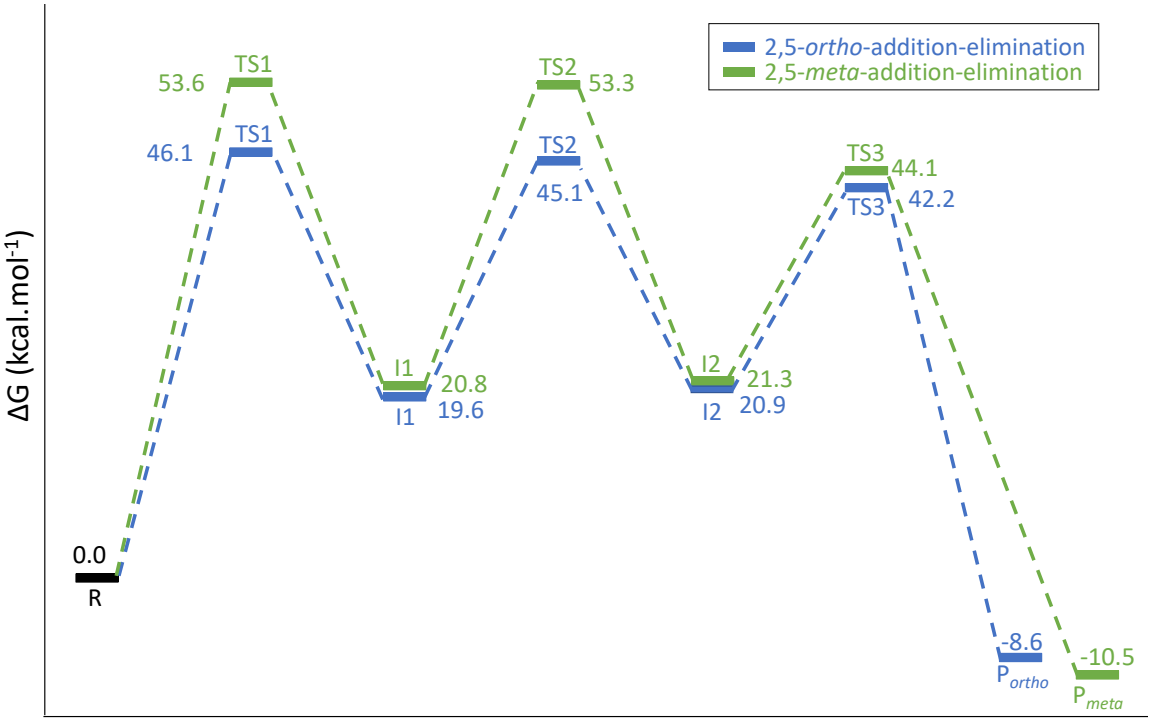


**Figure S5.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of anisole in the gas phase following a 2,5-addition-elimination pathway at the *ortho* (blue) or *meta* (green) position. The reactants (R) correspond to anisole, HBr and $Br_2$, while bromoanisole and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

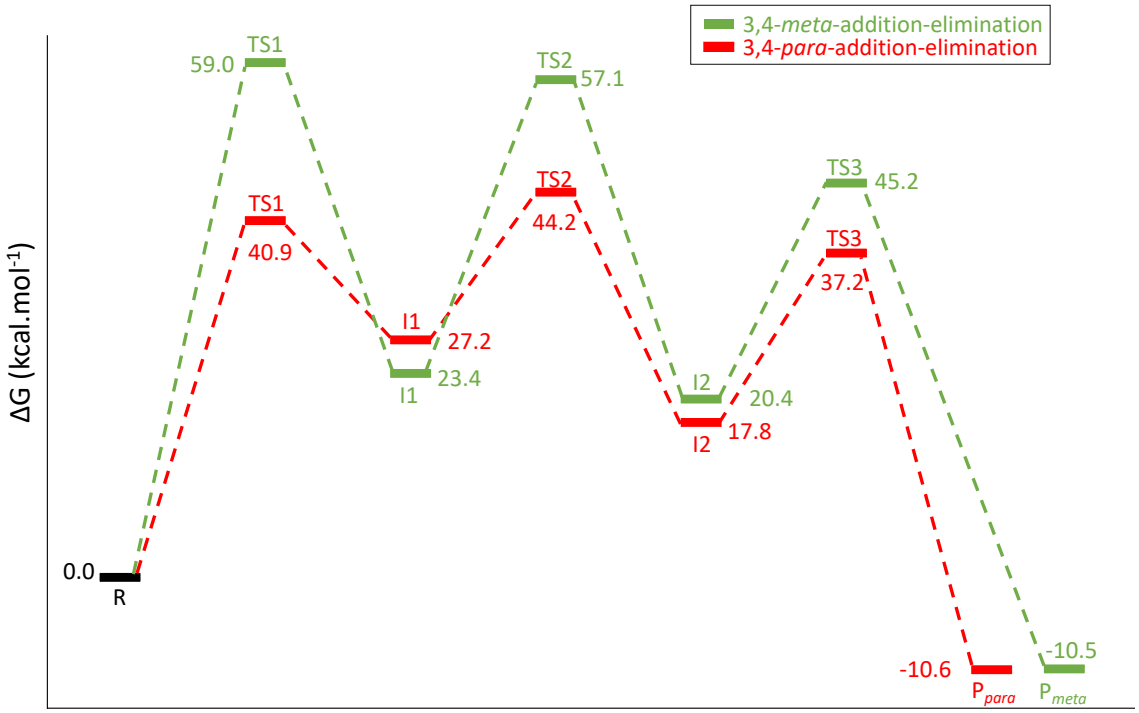


**Figure S6.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of anisole in the gas phase following a 3,4-addition-elimination pathway at the *meta* (green) or *para* (red) position. The reactants (R) correspond to anisole, HBr and $Br_2$, while bromoanisole and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

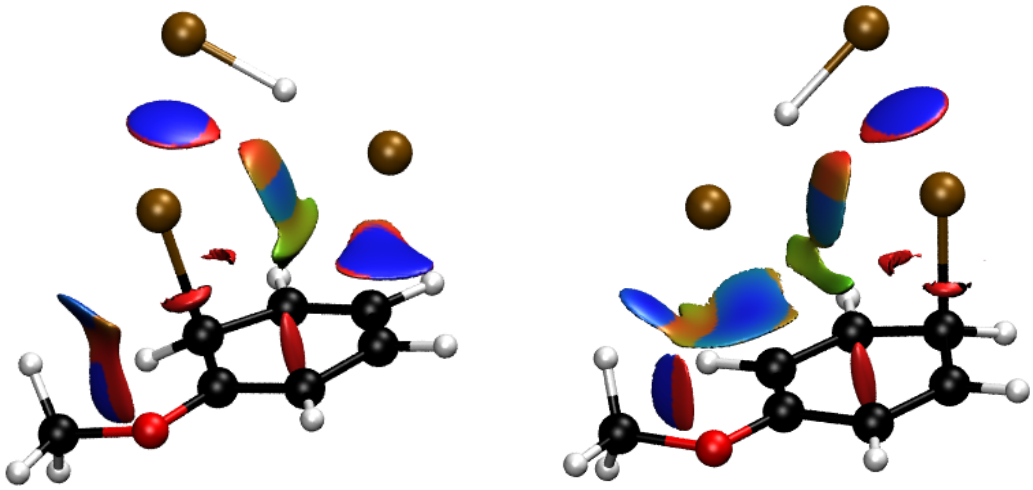


**Figure S7.** Non-covalent interactions present in the transition state describing the addition of bromine at the *ortho* (left) and *para* (right) position of anisole through a 2,5-addition-elimination and 3,4-addition-elimination pathway, respectively. The gradient isosurfaces ($s$ = 0.5) are coloured on a RGB scale according to the sign($\lambda_2$)$\rho$ over the range -0.01 a.u. to 0.01 a.u..

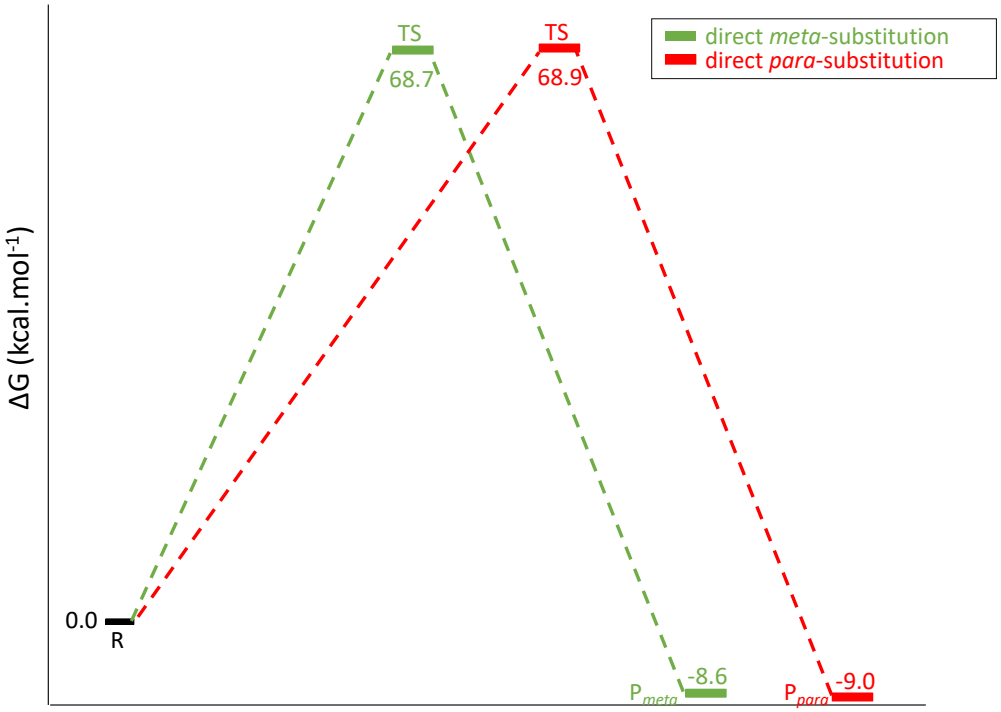


**Figure S8.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of nitrobenzene in the gas phase following a direct concerted substitution pathway at the *meta* (green) or *para* (red) position. The substitution at the *ortho* position could not be retrieved at this level of theory. The reactants (R) correspond to nitrobenzene, HBr and $Br_2$, while bromonitrobenzene and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

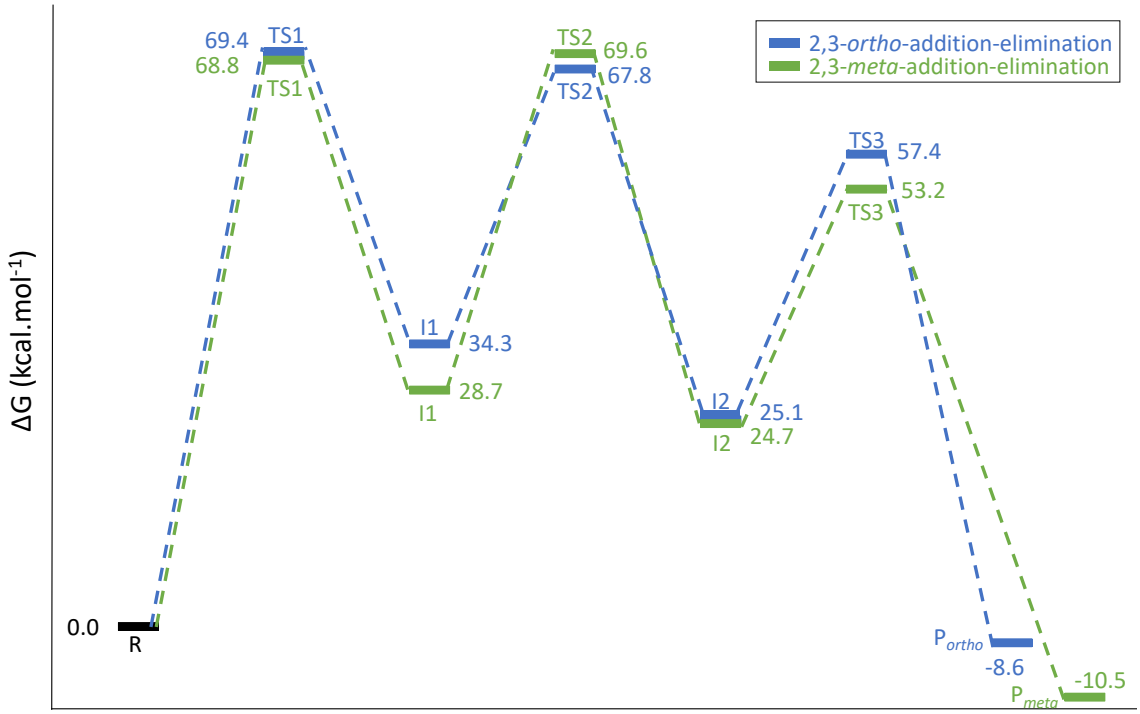


**Figure S9.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of nitrobenzene in the gas phase following a 2,3-addition-elimination pathway at the *ortho* (blue) or *meta* (green) position. The reactants (R) correspond to nitrobenzene, HBr and $Br_2$, while bromonitrobenzene and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

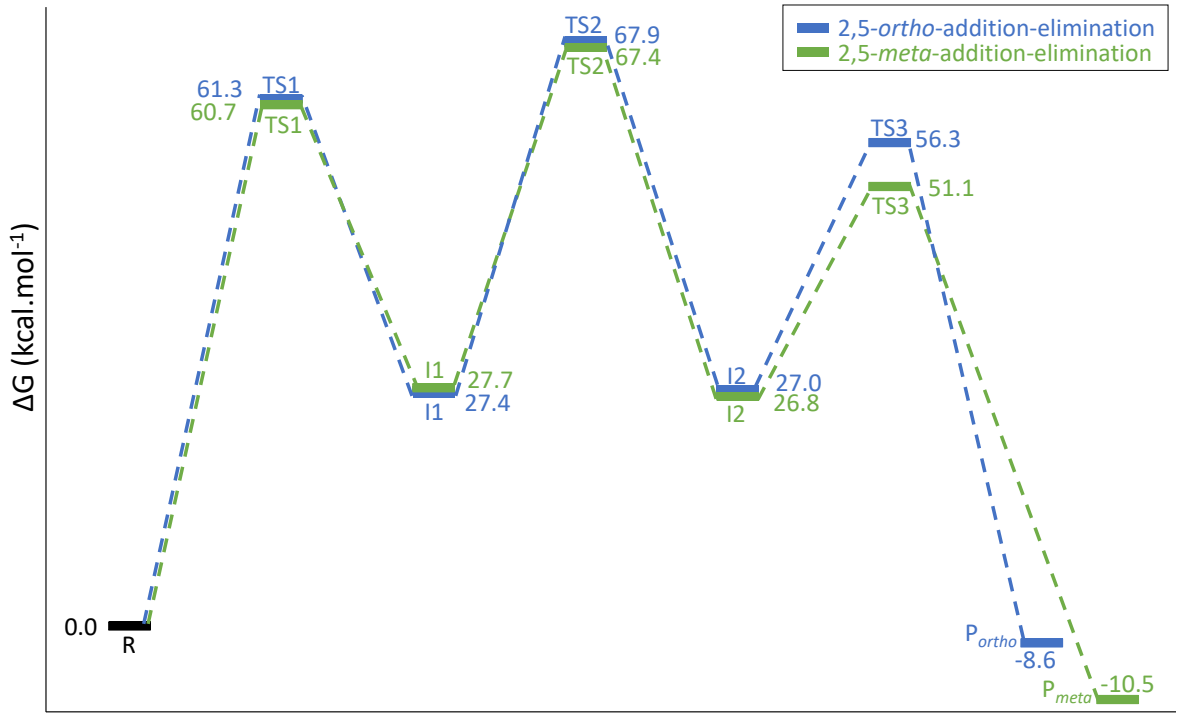


**Figure S10.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of nitrobenzene in the gas phase following a 2,5-addition-elimination pathway at the *ortho* (blue) or *meta* (green) position. The reactants (R) correspond to nitrobenzene, HBr and $Br_2$, while bromonitrobenzene and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

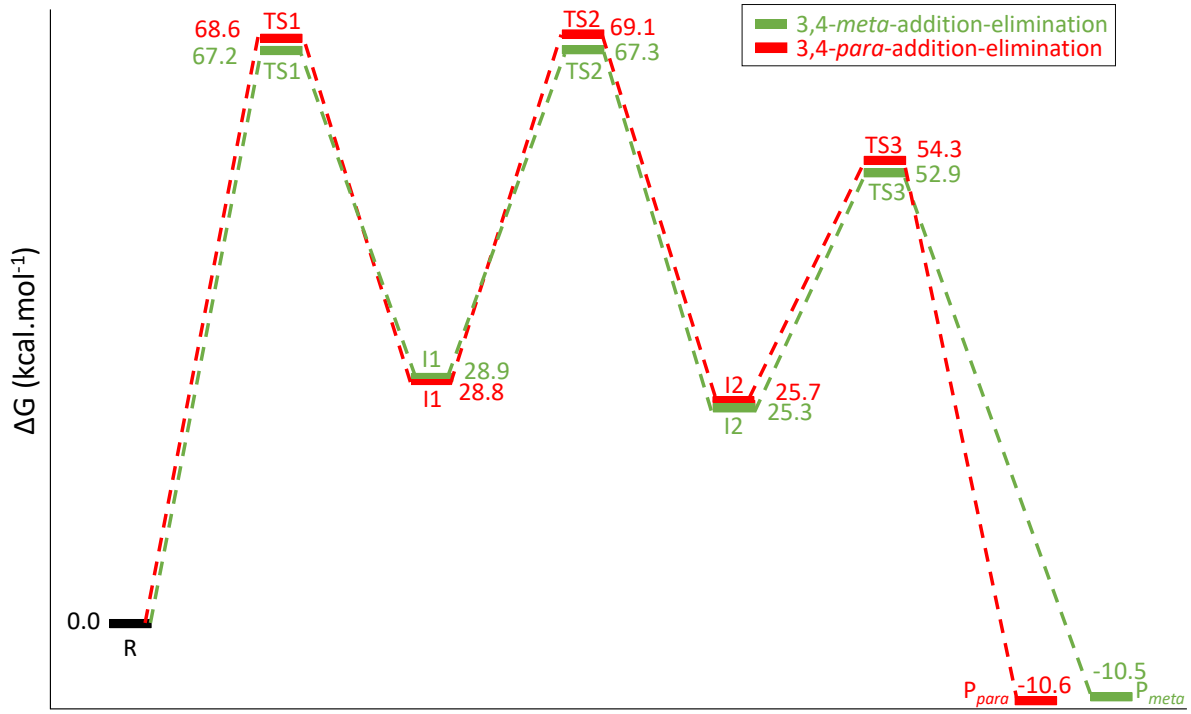


**Figure S11.** Gibbs free reaction profiles (in kcal.mol$^{-1}$) for the HBr assisted bromination of nitrobenzene in the gas phase following a 3,4-addition-elimination pathway at the *meta* (green) or *para* (red) position. The reactants (R) correspond to nitrobenzene, HBr and $Br_2$, while bromonitrobenzene and 2 HBr molecules are obtained as products (P). The transition states are indicated with "*TS*", the intermediate states are labelled as "*I*".

**Table S1.** Relative Gibbs free energies ($\Delta G^{\ddagger}$, in kcal.mol$^{-1}$) for the rate-determining transition state of the HBr-assisted bromination of benzene, methoxybenzene and nitrobenzene in gas phase together with differences in activation energies with respect to the most advantageous transition state ($\Delta\Delta G^{\ddagger}$, in kcal.mol$^{-1}$) determined at the ωB97X-D/cc-pVTZ and DLPNO-CCSD(T)/cc-pVTZ level of theory.

| | Mechanism | $\Delta G^{\ddagger}$ (DFT) | $\Delta\Delta G^{\ddagger}$ (DFT) | $\Delta G^{\ddagger}$ (DLPNO) | $\Delta\Delta G^{\ddagger}$ (DLPNO) |
|---|---|---|---|---|---|
| BENZENE | 1,4-*syn* add-elim | 53.3 | 0.0 | 57.2 | 0.0 |
| | 1,2-*cis* add-elim | 59.3 | 6.0 | 63.8 | 6.6 |
| | direct substitution | 59.5 | 6.2 | 64.3 | 7.1 |
| METHOXYBENZENE | Direct *ortho*-substitution | 49.7 | 8.8 | 54.5 | 10.3 |
| | Direct *meta*-substitution | 61.8 | 20.9 | 66.0 | 21.8 |
| | Direct *para*-substitution | 48.1 | 7.2 | 52.8 | 8.5 |
| | 2,3-*ortho* add-elim | 51.3 | 10.4 | 55.3 | 11.0 |
| | 2,3-*meta* add-elim | 61.2 | 20.3 | 64.7 | 20.4 |
| | 2,5-*ortho* add-elim | 46.1 | 5.2 | 49.6 | 5.4 |
| | 2,5-*meta* add-elim | 53.6 | 12.7 | 56.8 | 12.6 |
| | 3,4-*meta* add-elim | 59.0 | 18.1 | 63.1 | 18.9 |
| | 3,4-*para* add-elim | 40.9 | 0.0 | 44.2 | 0.0 |
| NITROBENZENE | Direct *meta*-substitution | 68.7 | 8.0 | 72.6 | 9.7 |
| | Direct *para*-substitution | 68.9 | 8.2 | 73.5 | 10.6 |
| | 2,3-*ortho* add-elim | 69.4 | 8.7 | 72.8 | 9.8 |
| | 2,3-*meta* add-elim | 68.8 | 8.1 | 72.5 | 9.6 |
| | 2,5-*ortho* add-elim | 61.3 | 0.6 | 63.2 | 0.2 |
| | 2,5-*meta* add-elim | 60.7 | 0.0 | 62.9 | 0.0 |
| | 3,4-*meta* add-elim | 67.2 | 6.5 | 71.5 | 8.6 |
| | 3,4-*para* add-elim | 68.6 | 7.9 | 72.4 | 9.4 |

**Table S2.** Root-mean-square deviation for the bond distances in the addition transition state and subsequent addition intermediate in anisole and nitrobenzene.

| Pathway | RMSD (Anisole) | RMSD (Nitrobenzene) |
|---|---|---|
| 2,3-*ortho* addition-elimination | 0.3317 | 0.2990 |
| 2,3-*meta* addition-elimination | 0.3255 | 0.2712 |
| 2,5-*ortho* addition-elimination | 0.2820 | 0.2454 |
| 2,5-*meta* addition-elimination | 0.2787 | 0.2327 |
| 3,4-*meta* addition-elimination | 0.3297 | 0.2854 |
| 3,4-par*a* addition-elimination | 0.3471 | 0.2852 |

## XYZ coordinates

## Bromination of benzene in gas phase

**benzene**

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 1.38701 |
| C | 0.00000 | 1.20108 | 0.69356 |
| C | 0.00000 | 1.20108 | -0.69356 |
| C | 0.00000 | 0.00000 | -1.38701 |
| C | 0.00000 | -1.20108 | -0.69356 |
| C | 0.00000 | -1.20108 | 0.69356 |
| H | 0.00000 | 0.00000 | 2.46886 |
| H | 0.00000 | 2.13828 | 1.23380 |
| H | 0.00000 | 2.13828 | -1.23380 |
| H | 0.00000 | 0.00000 | -2.46886 |
| H | 0.00000 | -2.13828 | -1.23380 |
| H | 0.00000 | -2.13828 | 1.23380 |

**dibromine**

| | | | |
|---|---|---|---|
| Br | 0.00000 | 0.00000 | 1.14029 |
| Br | 0.00000 | 0.00000 | -1.14029 |

**bromobenzene + HBr**

| | | | |
|---|---|---|---|
| C | 1.74980 | -1.94108 | 0.93930 |
| C | 3.02765 | -1.10685 | -0.91244 |
| C | 1.03888 | -0.75199 | 0.99564 |
| C | 2.32445 | 0.08724 | -0.87087 |
| C | 1.33766 | 0.24751 | 0.08623 |
| C | 2.74261 | -2.12050 | -0.01083 |
| H | 1.52047 | -2.72889 | 1.64327 |
| H | 3.80030 | -1.24165 | -1.65668 |
| H | 0.26225 | -0.60913 | 1.73261 |
| H | 2.53968 | 0.87969 | -1.57251 |
| Br | 0.36101 | 1.87898 | 0.14630 |
| H | -1.77493 | 0.32053 | -0.18764 |
| H | 3.29288 | -3.05013 | -0.04982 |
| Br | -2.73149 | -0.73773 | -0.18262 |

**1,4-*syn* TS1**

| | | | |
|---|---|---|---|
| C | -1.27037 | 0.83483 | -1.10769 |
| C | -1.23483 | -0.87477 | 1.11201 |
| C | -1.24667 | -0.51547 | -1.30779 |
| C | -1.25687 | 0.47556 | 1.31211 |
| C | -1.18920 | 1.33724 | 0.20276 |
| C | -1.14328 | -1.37414 | -0.19889 |
| H | -1.29178 | 1.52200 | -1.94044 |
| H | -1.22791 | -1.56219 | 1.94480 |
| H | -1.24878 | -0.93194 | -2.30413 |
| H | -1.26817 | 0.89179 | 2.30850 |
| H | -1.19968 | 2.40436 | 0.36145 |
| H | -1.11709 | -2.44099 | -0.35762 |
| Br | 1.61270 | -1.46446 | -0.23740 |
| Br | 1.56101 | 1.52380 | 0.22665 |

**1,4-*syn* I1**

| | | | |
|---|---|---|---|
| C | -1.24862 | 0.66272 | 1.06833 |
| C | -1.24862 | -0.66272 | 1.06833 |
| C | 1.24862 | -0.66272 | 1.06833 |
| C | 1.24862 | 0.66272 | 1.06833 |
| C | 0.00000 | 1.46564 | 1.01977 |
| C | 0.00000 | -1.46564 | 1.01977 |
| H | -2.18070 | 1.21011 | 1.10502 |
| H | -2.18070 | -1.21011 | 1.10502 |
| H | 2.18070 | -1.21011 | 1.10502 |
| H | 2.18070 | 1.21011 | 1.10502 |
| H | 0.00000 | 2.24124 | 1.78179 |
| H | 0.00000 | -2.24124 | 1.78179 |
| Br | 0.00000 | -2.54582 | -0.65516 |
| Br | 0.00000 | 2.54582 | -0.65516 |

**1,4-*syn* TS2**

| | | | |
|---|---|---|---|
| C | 0.15693 | 1.84851 | -0.13602 |
| C | -0.82282 | 0.84170 | 0.04743 |
| C | -0.50314 | -0.41656 | 0.60151 |
| C | 1.43742 | 1.60790 | 0.21187 |
| C | 1.83917 | 0.31445 | 0.79510 |
| C | 0.77051 | -0.68845 | 0.95763 |
| H | -1.87168 | 0.98108 | -0.23047 |
| Br | -3.81390 | -0.25924 | -0.16317 |
| H | -0.13266 | 2.79797 | -0.56199 |
| H | 2.21124 | 2.35194 | 0.07907 |
| H | -1.31860 | -1.12187 | 0.70540 |
| H | 1.04995 | -1.64497 | 1.37800 |
| Br | 3.25501 | -0.45178 | -0.35056 |
| H | 2.35450 | 0.47614 | 1.74545 |

**1,4-*syn* TS3**

| | | | |
|---|---|---|---|
| C | -1.09318 | -1.47048 | 1.22792 |
| C | -1.09318 | -1.47048 | -1.22792 |
| C | -1.09318 | -0.12013 | 1.23652 |
| C | -1.09318 | -0.12013 | -1.23652 |
| C | -0.69736 | 0.53270 | 0.00000 |
| C | -0.81434 | -2.12364 | 0.00000 |
| H | -1.19372 | -2.04554 | 2.13553 |
| H | -1.19372 | -2.04554 | -2.13553 |
| H | -1.18300 | 0.45785 | 2.14401 |
| H | -1.18300 | 0.45785 | -2.14401 |
| Br | -0.69665 | 2.45093 | 0.00000 |
| H | 0.45184 | 0.12370 | 0.00000 |
| H | -0.64728 | -3.19042 | 0.00000 |
| Br | 1.84680 | -1.45449 | 0.00000 |

**1,4-*syn* I2**

| | | | |
|---|---|---|---|
| C | -0.00077 | 1.46689 | 0.00000 |
| C | -0.00077 | -0.66278 | 1.24843 |
| C | -0.00077 | -0.66278 | -1.24843 |
| C | 0.00077 | 0.66278 | -1.24843 |
| C | 0.00077 | -1.46689 | 0.00000 |
| C | 0.00077 | 0.66278 | 1.24843 |
| H | 0.80436 | 2.19835 | 0.00000 |
| H | -0.80436 | -2.19835 | 0.00000 |
| Br | -1.61264 | 2.63954 | 0.00000 |
| Br | 1.61264 | -2.63954 | 0.00000 |
| H | -0.00294 | 1.20904 | 2.18180 |
| H | 0.00294 | -1.20904 | 2.18180 |
| H | 0.00294 | -1.20904 | -2.18180 |
| H | -0.00294 | 1.20904 | -2.18180 |

**1,2-*cis* TS1***

| | | | |
|---|---|---|---|
| C | -1.43797 | 1.98524 | 0.07330 |
| C | -3.08430 | 0.28795 | -0.55189 |
| C | -2.53987 | 1.55780 | -0.68942 |
| C | -2.52499 | -0.60097 | 0.33737 |
| C | -0.84028 | 1.13610 | 0.95021 |
| C | -1.31703 | -0.23961 | 1.05717 |
| Br | -0.07144 | -1.32658 | -0.16189 |
| H | -1.06298 | 2.99108 | -0.04333 |
| H | -3.94936 | 0.00258 | -1.13188 |
| H | -2.99132 | 2.25014 | -1.38721 |
| H | -2.95690 | -1.57475 | 0.51398 |
| H | 0.00688 | 1.43522 | 1.54818 |
| H | -1.15525 | -0.72310 | 2.01313 |
| Br | 2.43074 | 0.49401 | -0.08307 |

**1,2-*cis* I1***

| | | | |
|---|---|---|---|
| C | -0.43425 | 0.93095 | 0.38195 |
| C | 0.65577 | 0.00322 | 0.89374 |
| C | 2.21005 | 1.78140 | 0.20905 |
| C | 1.26109 | 2.19600 | -0.81664 |
| C | 0.00167 | 1.76387 | -0.78289 |
| C | 1.94090 | 0.75443 | 1.01748 |
| H | -0.65022 | 1.60351 | 1.21780 |
| H | 0.34970 | -0.44739 | 1.83099 |
| H | 3.16384 | 2.28665 | 0.27385 |
| H | 1.59571 | 2.85393 | -1.60651 |
| Br | 0.98612 | -1.56150 | -0.27900 |
| Br | -2.13504 | 0.03828 | 0.06950 |
| H | -0.72828 | 2.05081 | -1.52484 |
| H | 2.67005 | 0.38580 | 1.72508 |

**1,2-*cis* I2***

| | | | |
|---|---|---|---|
| C | -0.14730 | 1.41248 | 1.09697 |
| C | 0.14730 | -1.41248 | 1.09697 |
| C | 0.13605 | -0.71450 | 2.23298 |
| C | -0.13605 | 0.71450 | 2.23298 |
| C | 0.13605 | 0.74727 | -0.19974 |
| C | -0.13605 | -0.74727 | -0.19974 |
| H | -0.31324 | 2.48007 | 1.08879 |
| H | 0.31324 | -2.48007 | 1.08879 |
| H | 0.31153 | -1.21008 | 3.17768 |
| H | -0.31153 | 1.21008 | 3.17768 |
| H | -0.36312 | 1.22868 | -1.03179 |
| H | 0.36312 | -1.22868 | -1.03179 |
| Br | 2.06634 | 1.01815 | -0.62903 |
| Br | -2.06634 | -1.01815 | -0.62903 |

**1,2-*cis* TS2***

| | | | |
|---|---|---|---|
| C | -2.39134 | 1.19675 | 0.51996 |
| C | -2.06234 | 2.35115 | -0.09047 |
| C | -1.36278 | 0.17767 | 0.79163 |
| C | -0.71340 | 2.58816 | -0.48085 |
| C | 0.01199 | 0.49405 | 0.38562 |
| C | 0.30210 | 1.68106 | -0.24556 |
| Br | -1.85601 | -1.45830 | -0.20832 |
| H | -3.40768 | 0.98003 | 0.81756 |
| H | -2.81326 | 3.09962 | -0.29704 |
| H | -1.38545 | -0.15392 | 1.83203 |
| H | -0.48177 | 3.51863 | -0.98389 |
| H | 0.83485 | -0.20348 | 0.56454 |
| H | 1.33043 | 1.85184 | -0.53854 |
| Br | 3.09079 | -0.25672 | 0.01756 |

**1,2-*cis* TS3***

| | | | |
|---|---|---|---|
| C | -0.66098 | 1.82163 | 1.24399 |
| C | 0.27384 | 2.56409 | -0.89246 |
| C | -0.13346 | 0.55831 | 1.04274 |
| C | 0.86398 | 1.36194 | -1.09057 |
| C | 0.62936 | 0.26838 | -0.16528 |
| C | -0.47016 | 2.79467 | 0.28899 |
| H | -1.22988 | 2.02938 | 2.13730 |
| H | 0.38955 | 3.35868 | -1.61451 |
| H | -0.22022 | -0.21401 | 1.78978 |
| H | 1.46443 | 1.16434 | -1.96714 |
| Br | 2.13722 | -0.91698 | 0.10017 |
| H | -0.17841 | -0.39017 | -0.67264 |
| H | -0.89419 | 3.77742 | 0.44896 |
| Br | -2.20427 | -0.96701 | -0.17691 |

## HBr-assisted bromination of benzene in gas phase

**bromobenzene + 2HBr**

| | | | |
|---|---|---|---|
| C | -0.35981 | -1.81963 | 1.03884 |
| C | 0.55514 | -1.27983 | 1.92953 |
| C | 1.75026 | -0.74262 | 1.46979 |
| C | 2.01693 | -0.75723 | 0.10859 |
| C | 1.11218 | -1.29520 | -0.79313 |
| C | -0.07822 | -1.82538 | -0.31918 |
| Br | 3.64027 | -0.01592 | -0.52843 |
| H | 2.46579 | -0.31946 | 2.15956 |
| H | 0.18120 | 1.06942 | 0.61407 |
| H | 1.33211 | -1.29356 | -1.85049 |
| H | -0.79371 | -2.23639 | -1.01757 |
| Br | -0.71684 | 2.10856 | 0.23070 |
| Br | -3.76716 | -0.59856 | -0.40813 |
| H | -2.68149 | 0.30263 | -0.19420 |
| H | 0.34202 | -1.26890 | 2.98938 |
| H | -1.29415 | -2.22697 | 1.39775 |

**1,4-*syn* TS1**

| | | | |
|---|---|---|---|
| C | 2.48147 | 0.59951 | 1.22690 |
| C | 2.40922 | -0.75558 | -1.23387 |
| C | 2.40927 | -0.75580 | 1.23396 |
| C | 2.48140 | 0.59973 | -1.22659 |
| C | 2.43995 | 1.28867 | 0.00021 |
| C | 2.23501 | -1.49259 | -0.00002 |
| H | 2.52232 | 1.15765 | 2.14943 |
| H | 2.40184 | -1.30814 | -2.16297 |
| H | 2.40194 | -1.30852 | 2.16296 |
| H | 2.52218 | 1.15803 | -2.14902 |
| H | 2.50139 | 2.36594 | 0.00030 |
| H | 2.53074 | -2.53357 | -0.00012 |
| Br | 0.11305 | -1.59524 | -0.00017 |
| Br | -0.39570 | 2.15668 | -0.00008 |
| Br | -2.57611 | -0.48275 | 0.00013 |
| H | -1.56165 | 0.81066 | -0.00003 |

**Direct substitution TS**

| | | | |
|---|---|---|---|
| C | -3.95557 | -0.51903 | -0.75301 |
| C | -3.36052 | 0.46557 | 1.41063 |
| C | -4.27451 | -0.16651 | 0.55667 |
| C | -2.10977 | 0.75439 | 0.95098 |
| C | -2.70490 | -0.23186 | -1.23669 |
| C | -1.71819 | 0.40811 | -0.39967 |
| Br | -0.39516 | -1.10455 | -0.14890 |
| H | -4.68536 | -1.01644 | -1.37393 |
| H | -3.64966 | 0.71634 | 2.42020 |
| H | -5.26384 | -0.39627 | 0.93155 |
| H | -1.35959 | 1.24854 | 1.55591 |
| H | -2.42246 | -0.48263 | -2.24963 |
| H | -1.01821 | 1.13700 | -0.84359 |
| Br | 2.72692 | -1.08655 | 0.22530 |
| H | 2.11762 | 0.38711 | 0.04262 |
| Br | 1.24030 | 2.02374 | -0.18087 |

**1,4-*syn* I1**

| | | | |
|---|---|---|---|
| C | 0.08591 | -0.89687 | 1.62124 |
| C | -2.15432 | -1.62826 | 0.05908 |
| C | -0.96055 | -0.08293 | 1.61597 |
| C | -1.10576 | -2.43921 | 0.05856 |
| C | 0.15048 | -2.11891 | 0.78140 |
| C | -2.16337 | -0.33007 | 0.78062 |
| H | 0.94607 | -0.67816 | 2.23942 |
| H | -3.05188 | -1.89308 | -0.48304 |
| H | -0.96255 | 0.80825 | 2.22853 |
| H | -1.13515 | -3.37416 | -0.48421 |
| H | 0.52055 | -2.97322 | 1.34176 |
| H | -3.07666 | -0.20377 | 1.35653 |
| Br | -2.31428 | 1.13547 | -0.55896 |
| Br | 1.60902 | -1.87161 | -0.56908 |
| Br | 1.90747 | 2.23287 | 0.11601 |
| H | 1.56809 | 0.90607 | -0.27904 |

**1,4-*syn* TS2**

| | | | |
|---|---|---|---|
| C | 1.47880 | -0.58701 | -1.04251 |
| C | -0.10115 | -0.41907 | 0.73667 |
| C | 0.21534 | -0.34695 | -0.63945 |
| C | 0.87199 | -0.74380 | 1.71457 |
| C | 2.53773 | -0.94491 | -0.08166 |
| C | 2.14147 | -0.99127 | 1.33718 |
| H | 1.75572 | -0.53461 | -2.08636 |
| H | -1.11233 | -0.21603 | 1.04690 |
| H | 0.58128 | -0.78241 | 2.75363 |
| H | 2.99573 | -1.89617 | -0.36680 |
| H | 2.90894 | -1.23836 | 2.05822 |
| Br | -2.29514 | 1.89424 | 0.09170 |
| H | -2.80436 | 0.25700 | -0.11996 |
| Br | 4.01944 | 0.34231 | -0.25313 |
| Br | -3.05627 | -1.41658 | -0.24150 |
| H | -0.57113 | -0.09022 | -1.33169 |

**1,4-*syn* TS3**

| | | | |
|---|---|---|---|
| C | 0.75260 | 2.19279 | -0.00017 |
| C | 0.15744 | 1.84266 | 1.22932 |
| C | -0.94407 | 1.05507 | 1.23954 |
| C | -1.44244 | 0.48640 | -0.00001 |
| C | -0.94397 | 1.05470 | -1.23968 |
| C | 0.15763 | 1.84219 | -1.22961 |
| Br | -3.30397 | -0.01615 | 0.00003 |
| H | -1.40789 | 0.74712 | 2.16579 |
| H | -0.85338 | -0.52319 | 0.00010 |
| H | -1.40780 | 0.74660 | -2.16588 |
| H | 0.60081 | 2.18677 | -2.15117 |
| Br | 0.65946 | -2.07216 | 0.00003 |
| Br | 3.00518 | 0.42561 | 0.00006 |
| H | 1.82728 | -0.86002 | 0.00001 |
| H | 0.60049 | 2.18759 | 2.15082 |
| H | 1.59385 | 2.86701 | -0.00023 |

**1,4-*syn* I2**

| | | | |
|---|---|---|---|
| C | 1.42701 | -0.35561 | 1.14457 |
| C | -0.24581 | 0.53826 | -0.43014 |
| C | 0.17186 | -0.29742 | 0.72239 |
| C | 0.85524 | 1.28528 | -1.08657 |
| C | 2.52884 | 0.40454 | 0.50088 |
| C | 2.10991 | 1.22707 | -0.66282 |
| H | 1.69141 | -0.98259 | 1.98507 |
| H | -0.82789 | -0.03587 | -1.14777 |
| H | 0.59356 | 1.89657 | -1.93940 |
| H | 3.07502 | 1.00077 | 1.22873 |
| H | 2.88438 | 1.78454 | -1.17169 |
| Br | -3.59093 | -1.53751 | -0.14649 |
| H | -3.23644 | -0.17237 | 0.08572 |
| Br | 3.92174 | -0.88326 | -0.10212 |
| Br | -1.60687 | 1.86562 | 0.20903 |
| H | -0.60006 | -0.87363 | 1.21442 |

**1,2-*cis* TS1***

| | | | |
|---|---|---|---|
| C | 2.89745 | -1.43170 | 0.06859 |
| C | 3.38348 | 0.68106 | 1.07310 |
| C | 3.51147 | -0.72274 | 1.04873 |
| C | 2.64836 | 1.38236 | 0.13071 |
| C | 2.05902 | -0.76124 | -0.91566 |
| C | 1.99774 | 0.69584 | -0.86534 |
| H | 2.97374 | -2.50833 | 0.01539 |
| H | 3.88357 | 1.23218 | 1.85902 |
| H | 4.09530 | -1.22108 | 1.80801 |
| H | 2.55668 | 2.45581 | 0.18784 |
| H | 2.11333 | -1.16666 | -1.92219 |
| H | 1.44847 | 1.21850 | -1.63317 |
| Br | -0.72690 | 2.09416 | -0.11936 |
| H | -1.91876 | 0.58289 | 0.16727 |
| Br | 0.19027 | -1.34164 | -0.34960 |
| Br | -2.72445 | -0.74266 | 0.36259 |

**1,2-*cis* I1***

| | | | |
|---|---|---|---|
| C | 2.53153 | 1.42160 | -0.17339 |
| C | 0.59438 | 2.84534 | -0.45975 |
| C | 1.98436 | 2.63240 | -0.07726 |
| C | -0.23730 | 1.81529 | -0.62845 |
| C | 1.71702 | 0.31626 | -0.76960 |
| C | 0.24054 | 0.41593 | -0.43103 |
| H | 3.55939 | 1.22834 | 0.09462 |
| H | 0.22921 | 3.85804 | -0.56057 |
| H | 2.56362 | 3.46986 | 0.28568 |
| H | -1.28801 | 1.95907 | -0.83838 |
| H | 1.76127 | 0.41123 | -1.85911 |
| H | -0.33094 | -0.30263 | -1.00819 |
| Br | -0.16634 | -0.09853 | 1.45389 |
| H | -2.56470 | -0.37845 | 0.50524 |
| Br | 2.47828 | -1.44219 | -0.43506 |
| Br | -3.59518 | -0.37147 | -0.48689 |

**1,2-*cis* I2***

| | | | |
|---|---|---|---|
| C | 2.61276 | 1.18453 | 0.29710 |
| C | 1.11676 | 0.92050 | 2.19097 |
| C | 2.30222 | 1.47928 | 1.56005 |
| C | 0.18210 | 0.29769 | 1.47188 |
| C | 1.75866 | 0.26283 | -0.49418 |
| C | 0.32621 | 0.17566 | 0.00096 |
| H | 3.51109 | 1.56229 | -0.16940 |
| H | 0.99532 | 1.03200 | 3.25943 |
| H | -0.71743 | -0.09701 | 1.92229 |
| H | 1.78725 | 0.47767 | -1.55554 |
| H | -0.17285 | -0.70015 | -0.39688 |
| Br | -3.43225 | -0.98600 | 0.23956 |
| H | -2.76818 | 0.17206 | -0.26959 |
| Br | 2.54690 | -1.56439 | -0.39120 |
| Br | -0.69673 | 1.67912 | -0.85102 |
| H | 2.94544 | 2.12464 | 2.14188 |

**1,2-*cis* TS2***

| | | | |
|---|---|---|---|
| C | 2.85876 | 1.52771 | 0.14637 |
| C | 1.17636 | 2.03439 | 1.77556 |
| C | 2.50955 | 2.15042 | 1.28658 |
| C | 0.19517 | 1.31350 | 1.12794 |
| C | 1.86727 | 0.73606 | -0.60087 |
| C | 0.51175 | 0.66007 | -0.04173 |
| H | 3.86168 | 1.58407 | -0.25248 |
| H | 0.92705 | 2.53635 | 2.70194 |
| H | -0.80926 | 1.24009 | 1.51507 |
| H | 1.80286 | 1.06729 | -1.64171 |
| H | -0.23232 | 0.09765 | -0.58318 |
| Br | -1.61329 | -1.63334 | 0.91979 |
| H | -2.25392 | -0.33477 | 0.00923 |
| Br | 2.52160 | -1.11432 | -0.74124 |
| Br | -2.65797 | 1.04891 | -0.91442 |
| H | 3.22887 | 2.73250 | 1.84341 |

**1,2-*cis* TS3***

| | | | |
|---|---|---|---|
| C | -1.02633 | 2.85620 | 1.09242 |
| C | -1.51506 | 1.83832 | 1.94985 |
| C | -1.60350 | 0.56964 | 1.49681 |
| C | -1.12036 | 0.21980 | 0.16545 |
| C | -0.60145 | 1.29732 | -0.65967 |
| C | -0.57764 | 2.59670 | -0.18084 |
| Br | -2.38869 | -0.88489 | -0.82340 |
| H | -1.98041 | -0.23178 | 2.11621 |
| H | -0.27300 | -0.53284 | 0.34125 |
| H | -0.34796 | 1.07700 | -1.68426 |
| H | -0.19749 | 3.39006 | -0.80574 |
| Br | 1.29420 | -1.96390 | 0.68773 |
| Br | 2.30606 | 0.98085 | -0.65284 |
| H | 1.90224 | -0.55854 | 0.03860 |
| H | -1.83139 | 2.09039 | 2.95116 |
| H | -1.01119 | 3.87541 | 1.45615 |

## HBr-assisted bromination of benzene in $CCl_4$

**benzene**

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 1.38732 |
| C | 0.00000 | 1.20148 | 0.69375 |
| C | 0.00000 | 1.20148 | -0.69375 |
| C | 0.00000 | 0.00000 | -1.38732 |
| C | 0.00000 | -1.20148 | -0.69375 |
| C | 0.00000 | -1.20148 | 0.69375 |
| H | 0.00000 | 0.00000 | 2.46947 |
| H | 0.00000 | 2.13897 | 1.23398 |
| H | 0.00000 | 2.13897 | -1.23398 |
| H | 0.00000 | 0.00000 | -2.46947 |
| H | 0.00000 | -2.13897 | -1.23398 |
| H | 0.00000 | -2.13897 | 1.23398 |

**dibromine**

| | | | |
|---|---|---|---|
| Br | 0.00000 | 0.00000 | 1.14129 |
| Br | 0.00000 | 0.00000 | -1.14129 |

**HBr**

| | | | |
|---|---|---|---|
| Br | 0.00000 | 0.00000 | 0.03943 |
| H | 0.00000 | 0.00000 | -1.38011 |

**bromobenzene + 2HBr**

| | | | |
|---|---|---|---|
| C | -0.16330 | -1.99955 | 1.11056 |
| C | 0.72117 | -1.35503 | 1.96225 |
| C | 1.85276 | -0.72818 | 1.45675 |
| C | 2.08438 | -0.75835 | 0.08932 |
| C | 1.21020 | -1.39874 | -0.77434 |
| C | 0.08427 | -2.01969 | -0.25394 |
| Br | 3.62060 | 0.10882 | -0.61216 |
| H | 2.54247 | -0.22493 | 2.11873 |
| H | 0.13419 | 0.91751 | 0.67897 |
| H | 1.40057 | -1.41005 | -1.83760 |
| H | -0.60392 | -2.51665 | -0.92366 |
| Br | -0.71946 | 2.00742 | 0.33274 |
| Br | -3.89932 | -0.50778 | -0.46137 |
| H | -2.76310 | 0.31019 | -0.18811 |
| H | 0.53445 | -1.33276 | 3.02703 |
| H | -1.04502 | -2.48189 | 1.50835 |

**Direct substitution TS**

| | | | |
|---|---|---|---|
| C | -4.13875 | -0.54717 | -0.40744 |
| C | -3.18051 | 0.83809 | 1.38412 |
| C | -4.22265 | 0.07467 | 0.84334 |
| C | -2.02955 | 0.98808 | 0.67159 |
| C | -2.99996 | -0.40639 | -1.14441 |
| C | -1.86947 | 0.34620 | -0.62599 |
| Br | -0.52158 | -1.09779 | -0.23059 |
| H | -4.96871 | -1.12952 | -0.77778 |
| H | -3.29243 | 1.29453 | 2.35591 |
| H | -5.13157 | -0.04448 | 1.41953 |
| H | -1.18487 | 1.56235 | 1.03350 |
| H | -2.90132 | -0.85902 | -2.12146 |
| H | -1.32099 | 0.95151 | -1.34671 |
| Br | 2.69692 | -1.17097 | 0.31911 |
| H | 2.12886 | 0.38427 | 0.05610 |
| Br | 1.46227 | 1.98531 | -0.22985 |

**1,4-*syn* TS1**

| | | | |
|---|---|---|---|
| C | 2.49884 | 0.84619 | 1.22922 |
| C | 2.49884 | -0.51089 | -1.23933 |
| C | 2.49884 | -0.51089 | 1.23933 |
| C | 2.49884 | 0.84619 | -1.22922 |
| C | 2.43636 | 1.52402 | 0.00000 |
| C | 2.38345 | -1.26380 | 0.00000 |
| H | 2.50677 | 1.40796 | 2.15042 |
| H | 2.51637 | -1.06408 | -2.16811 |
| H | 2.51637 | -1.06408 | 2.16811 |
| H | 2.50677 | 1.40796 | -2.15042 |
| H | 2.41303 | 2.60440 | 0.00000 |
| H | 2.82068 | -2.25536 | 0.00000 |
| Br | 0.34144 | -1.60759 | 0.00000 |
| Br | -0.68518 | 2.12137 | 0.00000 |
| Br | -2.58495 | -0.72249 | 0.00000 |
| H | -1.66678 | 0.68326 | 0.00000 |

**1,4-*syn* I1**

| | | | |
|---|---|---|---|
| C | -0.19822 | -0.95302 | 1.63644 |
| C | -2.47219 | -1.17822 | -0.03103 |
| C | -1.06915 | 0.04729 | 1.63396 |
| C | -1.59964 | -2.17663 | -0.03251 |
| C | -0.33615 | -2.13036 | 0.74381 |
| C | -2.25980 | 0.06816 | 0.74713 |
| H | 0.65481 | -0.93562 | 2.30174 |
| H | -3.38500 | -1.24810 | -0.60720 |
| H | -0.93389 | 0.89188 | 2.29597 |
| H | -1.79085 | -3.07132 | -0.60956 |
| H | -0.15524 | -3.06103 | 1.27454 |
| H | -3.15495 | 0.35050 | 1.29521 |
| Br | -2.06682 | 1.58921 | -0.53433 |
| Br | 1.19918 | -2.11254 | -0.55307 |
| Br | 2.42870 | 1.79302 | 0.11604 |
| H | 1.73905 | 0.57113 | -0.13997 |

**1,4-*syn* I2**

| | | | |
|---|---|---|---|
| C | 1.57712 | -0.38668 | 1.15720 |
| C | -0.13162 | 0.44121 | -0.41408 |
| C | 0.31590 | -0.36392 | 0.74835 |
| C | 0.94378 | 1.20170 | -1.09598 |
| C | 2.65320 | 0.38523 | 0.48625 |
| C | 2.20461 | 1.17824 | -0.68592 |
| H | 1.86223 | -0.98883 | 2.00921 |
| H | -0.71110 | -0.15276 | -1.11718 |
| H | 0.66049 | 1.79103 | -1.95752 |
| H | 3.19930 | 1.00258 | 1.19622 |
| H | 2.95864 | 1.74777 | -1.21222 |
| Br | -3.96871 | -1.35142 | -0.14842 |
| H | -3.26947 | -0.12034 | 0.05602 |
| Br | 4.06501 | -0.89297 | -0.11674 |
| Br | -1.51467 | 1.75675 | 0.22475 |
| H | -0.43492 | -0.94679 | 1.26477 |

**1,4-*syn* TS2**

| | | | |
|---|---|---|---|
| C | 1.56178 | -0.59312 | -1.00588 |
| C | 0.00626 | -0.44360 | 0.79123 |
| C | 0.29547 | -0.38024 | -0.58606 |
| C | 0.98917 | -0.72335 | 1.76378 |
| C | 2.63300 | -0.91953 | -0.05122 |
| C | 2.26372 | -0.94212 | 1.37289 |
| H | 1.82175 | -0.55058 | -2.05502 |
| H | -1.01276 | -0.26625 | 1.10478 |
| H | 0.71252 | -0.75188 | 2.80683 |
| H | 3.07079 | -1.88827 | -0.31997 |
| H | 3.04476 | -1.15889 | 2.08887 |
| Br | -2.40671 | 1.88918 | 0.09154 |
| H | -2.86232 | 0.23916 | -0.10958 |
| Br | 4.11584 | 0.35134 | -0.29120 |
| Br | -3.15962 | -1.42505 | -0.25607 |
| H | -0.50437 | -0.15283 | -1.27380 |

**1,4-*syn* TS3**

| | | | |
|---|---|---|---|
| C | -0.59560 | -2.24678 | 0.00020 |
| C | -0.03649 | -1.85359 | 1.23184 |
| C | 1.01640 | -1.00289 | 1.24480 |
| C | 1.49706 | -0.41618 | -0.00003 |
| C | 1.01658 | -1.00339 | -1.24468 |
| C | -0.03634 | -1.85406 | -1.23153 |
| Br | 3.36929 | 0.07326 | -0.00002 |
| H | 1.45493 | -0.66582 | 2.17387 |
| H | 0.92497 | 0.57313 | -0.00029 |
| H | 1.45525 | -0.66671 | -2.17382 |
| H | -0.45982 | -2.22559 | -2.15192 |
| Br | -0.81999 | 2.09536 | -0.00004 |
| Br | -3.02848 | -0.52260 | -0.00005 |
| H | -1.90719 | 0.81886 | -0.00005 |
| H | -0.46006 | -2.22478 | 2.15232 |
| H | -1.40685 | -2.95860 | 0.00028 |

**1,2-*cis* TS1***

| | | | |
|---|---|---|---|
| C | 3.15279 | -1.20902 | 0.10338 |
| C | 3.43201 | 0.95597 | 1.06505 |
| C | 3.72129 | -0.42287 | 1.04975 |
| C | 2.58568 | 1.56414 | 0.14164 |
| C | 2.22260 | -0.64563 | -0.87324 |
| C | 1.99416 | 0.79864 | -0.82214 |
| H | 3.34729 | -2.27175 | 0.05932 |
| H | 3.88608 | 1.56790 | 1.83429 |
| H | 4.38497 | -0.83941 | 1.79229 |
| H | 2.37615 | 2.62078 | 0.20180 |
| H | 2.37506 | -1.01625 | -1.88593 |
| H | 1.32490 | 1.23671 | -1.54875 |
| Br | -1.07181 | 2.08707 | -0.14960 |
| H | -2.01594 | 0.46567 | 0.14671 |
| Br | 0.44018 | -1.40162 | -0.36465 |
| Br | -2.74921 | -0.91434 | 0.38321 |

**1,2-*cis* TS2***

| | | | |
|---|---|---|---|
| C | 3.03663 | 1.38980 | 0.21523 |
| C | 1.36510 | 2.03861 | 1.79263 |
| C | 2.70987 | 2.04369 | 1.34978 |
| C | 0.33916 | 1.40309 | 1.10274 |
| C | 2.00511 | 0.69229 | -0.56681 |
| C | 0.63541 | 0.72330 | -0.04384 |
| H | 4.05215 | 1.36850 | -0.15551 |
| H | 1.12781 | 2.55373 | 2.71527 |
| H | -0.67935 | 1.43104 | 1.45922 |
| H | 1.99329 | 1.07789 | -1.59368 |
| H | -0.14406 | 0.22005 | -0.60032 |
| Br | -1.81964 | -1.63024 | 0.93496 |
| H | -2.28111 | -0.36728 | 0.07293 |
| Br | 2.52849 | -1.19277 | -0.76865 |
| Br | -2.65390 | 1.14902 | -0.93558 |
| H | 3.46025 | 2.56104 | 1.92856 |

**1,2-*cis* I1***

| | | | |
|---|---|---|---|
| C | 2.62567 | 1.43191 | 0.06784 |
| C | 0.71790 | 2.86338 | -0.34598 |
| C | 2.05369 | 2.62962 | 0.18583 |
| C | -0.07303 | 1.84509 | -0.69195 |
| C | 1.90352 | 0.37058 | -0.70120 |
| C | 0.39526 | 0.43754 | -0.54294 |
| H | 3.61903 | 1.22891 | 0.43978 |
| H | 0.35442 | 3.87940 | -0.41656 |
| H | 2.57379 | 3.44179 | 0.67445 |
| H | -1.09059 | 2.00468 | -1.02012 |
| H | 2.07882 | 0.54423 | -1.76766 |
| H | -0.09048 | -0.24000 | -1.23590 |
| Br | -0.23241 | -0.22233 | 1.24186 |
| H | -2.62729 | -0.32473 | 0.32922 |
| Br | 2.64388 | -1.40785 | -0.40332 |
| Br | -3.85592 | -0.31277 | -0.40519 |

**1,2-*cis* I2***

| | | | |
|---|---|---|---|
| C | 2.65652 | 1.28175 | 0.13908 |
| C | 1.25489 | 1.09247 | 2.11239 |
| C | 2.36910 | 1.67411 | 1.38124 |
| C | 0.34398 | 0.33726 | 1.49586 |
| C | 1.84662 | 0.22974 | -0.52456 |
| C | 0.44366 | 0.08640 | 0.03824 |
| H | 3.50418 | 1.67888 | -0.40085 |
| H | 1.16577 | 1.29605 | 3.17059 |
| H | -0.50337 | -0.07615 | 2.02410 |
| H | 1.82546 | 0.33923 | -1.60218 |
| H | -0.00711 | -0.85245 | -0.26079 |
| Br | -3.76510 | -0.85720 | 0.26559 |
| H | -2.80546 | 0.08023 | -0.22886 |
| Br | 2.77561 | -1.52370 | -0.28260 |
| Br | -0.71472 | 1.43530 | -0.90948 |
| H | 2.97951 | 2.41961 | 1.87181 |

**1,2-*cis* TS3***

| | | | |
|---|---|---|---|
| C | -1.35812 | 2.86213 | 0.74868 |
| C | -1.58603 | 1.91545 | 1.77143 |
| C | -1.49460 | 0.59610 | 1.48787 |
| C | -1.09908 | 0.14417 | 0.15573 |
| C | -0.80907 | 1.17678 | -0.83474 |
| C | -0.96958 | 2.50485 | -0.53266 |
| Br | -2.45965 | -1.06942 | -0.57684 |
| H | -1.68836 | -0.15958 | 2.23655 |
| H | -0.21860 | -0.54302 | 0.25579 |
| H | -0.52698 | 0.85788 | -1.82762 |
| H | -0.77683 | 3.26138 | -1.27754 |
| Br | 1.55287 | -1.98210 | 0.45178 |
| Br | 2.29089 | 1.21253 | -0.44397 |
| H | 2.00926 | -0.41295 | 0.00896 |
| H | -1.85446 | 2.25234 | 2.76150 |
| H | -1.48873 | 3.91162 | 0.98013 |

## HBr-assisted bromination of benzene in ACN

**benzene**

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 1.38867 |
| C | 0.00000 | 1.20265 | 0.69436 |
| C | 0.00000 | 1.20265 | -0.69436 |
| C | 0.00000 | 0.00000 | -1.38867 |
| C | 0.00000 | -1.20265 | -0.69436 |
| C | 0.00000 | -1.20265 | 0.69436 |
| H | 0.00000 | 0.00000 | 2.47092 |
| H | 0.00000 | 2.13987 | 1.23544 |
| H | 0.00000 | 2.13987 | -1.23544 |
| H | 0.00000 | 0.00000 | -2.47092 |
| H | 0.00000 | -2.13987 | -1.23544 |
| H | 0.00000 | -2.13987 | 1.23544 |

**dibromine**

| | | | |
|---|---|---|---|
| Br | 0.00000 | 0.00000 | 1.14141 |
| Br | 0.00000 | 0.00000 | -1.14141 |

**HBr**

| | | | |
|---|---|---|---|
| Br | 0.00000 | 0.00000 | 0.03947 |
| H | 0.00000 | 0.00000 | -1.38158 |

**bromobenzene + 2HBr**

| | | | |
|---|---|---|---|
| C | -0.20839 | -2.14707 | 0.65206 |
| C | 0.65591 | -1.73954 | 1.65811 |
| C | 1.81857 | -1.04778 | 1.35011 |
| C | 2.10018 | -0.77048 | 0.02130 |
| C | 1.24728 | -1.16747 | -0.99868 |
| C | 0.08844 | -1.86079 | -0.67225 |
| Br | 3.68385 | 0.18808 | -0.41394 |
| H | 2.48842 | -0.72795 | 2.13537 |
| H | 0.13432 | 0.79444 | 0.00930 |
| H | 1.47693 | -0.94291 | -2.03046 |
| H | -0.58083 | -2.17214 | -1.46244 |
| Br | -0.67551 | 1.92749 | 0.32758 |
| Br | -3.98695 | -0.40826 | -0.32060 |
| H | -2.79528 | 0.33406 | -0.06532 |
| H | 0.42822 | -1.95640 | 2.69272 |
| H | -1.11207 | -2.68609 | 0.90037 |

**1,4-*syn* I1**

| | | | |
|---|---|---|---|
| C | -0.26300 | -0.93726 | 1.65144 |
| C | -2.56352 | -1.00272 | 0.00345 |
| C | -1.05725 | 0.12587 | 1.64942 |
| C | -1.76644 | -2.06332 | 0.00045 |
| C | -0.49185 | -2.09832 | 0.75738 |
| C | -2.24292 | 0.23107 | 0.76301 |
| H | 0.58463 | -0.98874 | 2.32207 |
| H | -3.49340 | -1.01366 | -0.54941 |
| H | -0.86523 | 0.95500 | 2.31718 |
| H | -2.03558 | -2.95178 | -0.55496 |
| H | -0.35317 | -3.04296 | 1.27501 |
| H | -3.10948 | 0.60534 | 1.30089 |
| Br | -1.91005 | 1.70943 | -0.55326 |
| Br | 1.02354 | -2.15417 | -0.57605 |
| Br | 2.53983 | 1.60065 | 0.12877 |
| H | 1.71575 | 0.44773 | -0.04279 |

**1,4-*syn* TS1**

| | | | |
|---|---|---|---|
| C | 2.62163 | 1.18376 | 1.23391 |
| C | 2.62163 | -0.17168 | -1.24831 |
| C | 2.62163 | -0.17168 | 1.24831 |
| C | 2.62163 | 1.18376 | -1.23391 |
| C | 2.58823 | 1.85295 | 0.00000 |
| C | 2.56180 | -0.93740 | 0.00000 |
| H | 2.62737 | 1.75063 | 2.15201 |
| H | 2.63527 | -0.72539 | -2.17717 |
| H | 2.63527 | -0.72539 | 2.17717 |
| H | 2.62737 | 1.75063 | -2.15201 |
| H | 2.55356 | 2.93473 | 0.00000 |
| H | 3.21228 | -1.81053 | 0.00000 |
| Br | 0.69831 | -1.66214 | 0.00000 |
| Br | -1.06155 | 2.02143 | 0.00000 |
| Br | -2.72942 | -0.96967 | 0.00000 |
| H | -1.86739 | 0.55026 | 0.00000 |

**1,4-*syn* TS2**

| | | | |
|---|---|---|---|
| C | 1.66929 | -0.53775 | -1.01900 |
| C | 0.15589 | -0.53509 | 0.81707 |
| C | 0.40716 | -0.37822 | -0.55681 |
| C | 1.15374 | -0.87675 | 1.74626 |
| C | 2.76193 | -0.90399 | -0.10778 |
| C | 2.42699 | -1.04109 | 1.31584 |
| H | 1.90394 | -0.42343 | -2.06858 |
| H | -0.85536 | -0.38106 | 1.17124 |
| H | 0.89982 | -0.98877 | 2.78920 |
| H | 3.20875 | -1.84538 | -0.45468 |
| H | 3.22487 | -1.29844 | 1.99916 |
| Br | -2.58257 | 1.88609 | 0.13297 |
| H | -2.93662 | 0.24888 | -0.08388 |
| Br | 4.20362 | 0.42483 | -0.28621 |
| Br | -3.23504 | -1.44101 | -0.28411 |
| H | -0.40562 | -0.12144 | -1.21867 |

**1,4-*syn* I2**

| | | | |
|---|---|---|---|
| C | 1.60113 | -0.52000 | 1.08685 |
| C | -0.05595 | 0.42800 | -0.47034 |
| C | 0.35677 | -0.47732 | 0.62846 |
| C | 1.02965 | 1.26665 | -1.03227 |
| C | 2.68636 | 0.33048 | 0.53836 |
| C | 2.27359 | 1.22371 | -0.57252 |
| H | 1.86106 | -1.19390 | 1.89210 |
| H | -0.60509 | -0.09763 | -1.24761 |
| H | 0.77160 | 1.92857 | -1.84803 |
| H | 3.19675 | 0.88171 | 1.32480 |
| H | 3.03629 | 1.85503 | -1.00852 |
| Br | -4.14643 | -1.24376 | -0.15102 |
| H | -3.26122 | -0.13184 | 0.02682 |
| Br | 4.14425 | -0.87088 | -0.13155 |
| Br | -1.48201 | 1.66803 | 0.24640 |
| H | -0.40206 | -1.11963 | 1.05532 |

**1,2-*cis* TS1***

| | | | |
|---|---|---|---|
| C | 3.44507 | -1.04730 | 0.00303 |
| C | 3.87253 | 1.09953 | 0.93860 |
| C | 4.17881 | -0.26839 | 0.83465 |
| C | 2.84557 | 1.71353 | 0.20806 |
| C | 2.35327 | -0.47526 | -0.79096 |
| C | 2.09178 | 0.95926 | -0.63154 |
| H | 3.64960 | -2.10378 | -0.10672 |
| H | 4.45461 | 1.70662 | 1.62029 |
| H | 4.98406 | -0.68361 | 1.42108 |
| H | 2.65378 | 2.76856 | 0.33088 |
| H | 2.50391 | -0.70797 | -1.85125 |
| H | 1.27546 | 1.38844 | -1.19690 |
| Br | -1.50297 | 2.04230 | -0.14816 |
| H | -2.21495 | 0.43747 | 0.11016 |
| Br | 0.68313 | -1.41096 | -0.31241 |
| Br | -2.89527 | -1.05117 | 0.35490 |

**1,4-*syn* TS3**

| | | | |
|---|---|---|---|
| C | -0.30119 | -2.17099 | -0.02795 |
| C | 0.18579 | -1.72146 | 1.21415 |
| C | 1.15707 | -0.78110 | 1.24448 |
| C | 1.63971 | -0.16975 | 0.00180 |
| C | 1.16291 | -0.74996 | -1.25787 |
| C | 0.19086 | -1.69022 | -1.25601 |
| Br | 3.57065 | 0.10610 | 0.00891 |
| H | 1.55359 | -0.41521 | 2.18175 |
| H | 1.19753 | 0.84943 | 0.01275 |
| H | 1.56501 | -0.36134 | -2.18355 |
| H | -0.20040 | -2.08601 | -2.18053 |
| Br | -1.15755 | 2.05882 | -0.00250 |
| Br | -3.12605 | -0.73206 | 0.00980 |
| H | -2.12972 | 0.66920 | 0.00361 |
| H | -0.20990 | -2.14030 | 2.12657 |
| H | -1.03375 | -2.96492 | -0.03959 |

**1,2-*cis* I1***

| | | | |
|---|---|---|---|
| C | 2.68576 | 1.37343 | 0.08789 |
| C | 0.84452 | 2.87706 | -0.37365 |
| C | 2.15737 | 2.59321 | 0.19016 |
| C | 0.02328 | 1.88903 | -0.73857 |
| C | 1.94005 | 0.33927 | -0.69467 |
| C | 0.43380 | 0.46632 | -0.57934 |
| H | 3.66558 | 1.13840 | 0.47769 |
| H | 0.52509 | 3.90702 | -0.45659 |
| H | 2.69887 | 3.38830 | 0.68407 |
| H | -0.97724 | 2.08631 | -1.09778 |
| H | 2.14755 | 0.49801 | -1.75778 |
| H | -0.06529 | -0.19427 | -1.27875 |
| Br | -0.26425 | -0.16317 | 1.20292 |
| H | -2.60411 | -0.26477 | 0.27090 |
| Br | 2.60247 | -1.46840 | -0.36668 |
| Br | -3.87820 | -0.30526 | -0.38460 |

**1,2-*cis* TS2***

| | | | |
|---|---|---|---|
| C | 1.67348 | 1.38979 | -0.81376 |
| C | 1.46032 | 2.71777 | 1.14927 |
| C | 1.70711 | 2.61283 | -0.22684 |
| C | 1.17743 | 1.61047 | 1.96247 |
| C | 1.30421 | 0.20830 | -0.03629 |
| C | 1.14317 | 0.37255 | 1.40763 |
| H | 1.85376 | 1.27004 | -1.87345 |
| H | 1.49723 | 3.69785 | 1.60707 |
| H | 1.00684 | 1.74784 | 3.01932 |
| H | 0.26554 | -0.01534 | -0.37687 |
| H | 0.93227 | -0.50599 | 2.00159 |
| Br | -1.84599 | -1.83199 | 0.45445 |
| H | -2.02976 | -0.29018 | -0.05538 |
| Br | 2.33661 | -1.36824 | -0.51434 |
| Br | -2.09779 | 1.40389 | -0.63079 |
| H | 1.93089 | 3.49743 | -0.80324 |

**1,2-*cis* TS3***

| | | | |
|---|---|---|---|
| C | -2.13300 | 2.57071 | -0.07280 |
| C | -2.16074 | 1.96697 | 1.20114 |
| C | -1.66980 | 0.71577 | 1.35267 |
| C | -1.09259 | -0.00677 | 0.21193 |
| C | -1.00376 | 0.72744 | -1.05759 |
| C | -1.55207 | 1.96726 | -1.18827 |
| Br | -2.28052 | -1.55128 | -0.15123 |
| H | -1.70016 | 0.20836 | 2.30713 |
| H | -0.14279 | -0.48612 | 0.46363 |
| H | -0.53612 | 0.22722 | -1.89438 |
| H | -1.52571 | 2.48681 | -2.13349 |
| Br | 2.16304 | -1.73672 | 0.08950 |
| Br | 1.96357 | 1.68781 | -0.03253 |
| H | 2.13362 | -0.12830 | 0.02460 |
| H | -2.59390 | 2.49851 | 2.03460 |
| H | -2.57638 | 3.55174 | -0.18585 |

**1,2-*cis* I2***

| | | | |
|---|---|---|---|
| C | 2.69553 | 1.26813 | -0.05238 |
| C | 1.42310 | 1.26247 | 2.01705 |
| C | 2.49024 | 1.76860 | 1.16804 |
| C | 0.46918 | 0.46712 | 1.52707 |
| C | 1.83802 | 0.17291 | -0.56875 |
| C | 0.47514 | 0.09139 | 0.09390 |
| H | 3.50630 | 1.60981 | -0.68024 |
| H | 1.40493 | 1.55777 | 3.05724 |
| H | -0.34592 | 0.10931 | 2.14021 |
| H | 1.75492 | 0.18206 | -1.64908 |
| H | -0.00611 | -0.86060 | -0.09671 |
| Br | -3.83721 | -0.82084 | 0.27576 |
| H | -2.78568 | 0.04139 | -0.17089 |
| Br | 2.77020 | -1.56821 | -0.22217 |
| Br | -0.73325 | 1.37844 | -0.88970 |
| H | 3.13332 | 2.54788 | 1.55360 |

**Direct substitution TS**

| | | | |
|---|---|---|---|
| C | -4.33952 | -0.38866 | 0.58049 |
| C | -2.98781 | 1.67608 | 0.49012 |
| C | -4.08568 | 0.94013 | 0.95979 |
| C | -2.11328 | 1.08431 | -0.36225 |
| C | -3.48556 | -1.00532 | -0.27299 |
| C | -2.31790 | -0.29822 | -0.80614 |
| Br | -0.69306 | -1.29743 | -0.29715 |
| H | -5.20185 | -0.90375 | 0.97523 |
| H | -2.84047 | 2.69284 | 0.82096 |
| H | -4.76712 | 1.41642 | 1.65328 |
| H | -1.23622 | 1.60373 | -0.72848 |
| H | -3.64791 | -2.02570 | -0.59322 |
| H | -2.32958 | -0.33823 | -1.90163 |
| Br | 2.85492 | -1.14563 | 0.36850 |
| H | 2.26519 | 0.39066 | 0.09914 |
| Br | 1.65918 | 2.01774 | -0.18162 |

## HBr-assisted bromination of anisole in gas phase

**anisole**

| | | | |
|---|---|---|---|
| C | -0.91950 | -0.51304 | 0.00000 |
| C | 0.00000 | 0.52932 | 0.00000 |
| C | 1.36516 | 0.24713 | 0.00000 |
| C | 1.80020 | -1.06265 | 0.00000 |
| C | 0.88771 | -2.11145 | 0.00000 |
| C | -0.46454 | -1.82663 | 0.00000 |
| H | -1.98173 | -0.32067 | 0.00000 |
| H | 2.06428 | 1.07160 | 0.00000 |
| H | 2.86236 | -1.26816 | 0.00000 |
| H | 1.23209 | -3.13602 | 0.00000 |
| H | -1.18807 | -2.63095 | 0.00000 |
| O | -0.33228 | 1.84285 | 0.00000 |
| C | -1.69849 | 2.18218 | 0.00000 |
| H | -2.20532 | 1.80220 | 0.89123 |
| H | -1.74329 | 3.26775 | 0.00000 |
| H | -2.20532 | 1.80220 | -0.89123 |

***m*-bromoanisole**

| | | | |
|---|---|---|---|
| C | -1.83807 | 0.15925 | -0.00015 |
| C | -0.78360 | 2.31483 | 0.00012 |
| C | -1.93104 | 1.55060 | 0.00002 |
| C | 0.47456 | 1.72289 | 0.00011 |
| C | -0.59030 | -0.45370 | -0.00035 |
| C | 0.54464 | 0.34527 | -0.00014 |
| H | -0.86277 | 3.39338 | 0.00021 |
| H | 1.37279 | 2.32120 | 0.00013 |
| H | -0.48596 | -1.52673 | -0.00048 |
| Br | 2.24385 | -0.50081 | 0.00003 |
| H | -2.91096 | 2.00546 | 0.00012 |
| O | -3.00956 | -0.51271 | -0.00020 |
| C | -2.97659 | -1.92152 | 0.00030 |
| H | -2.47797 | -2.31036 | 0.89197 |
| H | -4.01280 | -2.24743 | 0.00062 |
| H | -2.47834 | -2.31101 | -0.89132 |

***o*-bromoanisole**

| | | | |
|---|---|---|---|
| C | -2.19607 | 0.08502 | -0.00018 |
| C | -1.56108 | -2.23568 | 0.00014 |
| C | -2.53876 | -1.25930 | -0.00001 |
| C | -0.22450 | -1.86187 | 0.00004 |
| C | -0.85896 | 0.47105 | -0.00015 |
| C | 0.12266 | -0.52564 | -0.00008 |
| Br | 1.94929 | -0.03631 | 0.00002 |
| H | -2.97547 | 0.83161 | -0.00010 |
| H | -1.82596 | -3.28320 | 0.00018 |
| H | 0.55481 | -2.61008 | 0.00013 |
| H | -3.58427 | -1.53546 | 0.00008 |
| O | -0.43905 | 1.74974 | -0.00034 |
| C | -1.40397 | 2.77571 | 0.00030 |
| H | -0.84884 | 3.70917 | 0.00029 |
| H | -2.03478 | 2.73281 | -0.89144 |
| H | -2.03413 | 2.73228 | 0.89246 |

***p*-bromoanisole**

| | | | |
|---|---|---|---|
| C | 1.44097 | -0.97901 | -0.00052 |
| C | 1.23103 | 1.41691 | -0.00017 |
| C | 2.03432 | 0.27740 | -0.00028 |
| C | -0.14325 | 1.30261 | -0.00010 |
| C | 0.05605 | -1.09149 | -0.00040 |
| C | -0.72819 | 0.04372 | -0.00012 |
| Br | -2.61861 | -0.11443 | 0.00014 |
| H | 2.03560 | -1.87970 | -0.00029 |
| H | 1.70638 | 2.38737 | 0.00017 |
| H | -0.76037 | 2.18944 | 0.00007 |
| H | -0.40233 | -2.06969 | -0.00039 |
| O | 3.36842 | 0.49591 | -0.00013 |
| C | 4.22845 | -0.61974 | 0.00062 |
| H | 4.08544 | -1.23562 | -0.89133 |
| H | 5.23893 | -0.22115 | 0.00124 |
| H | 4.08406 | -1.23543 | 0.89245 |

**Direct *ortho*-substitution TS**

| | | | |
|---|---|---|---|
| C | 3.70846 | -0.04750 | 0.48836 |
| C | 3.39360 | -0.75840 | -1.83815 |
| C | 4.19594 | -0.58271 | -0.69042 |
| C | 2.08049 | -0.40434 | -1.79517 |
| C | 2.37103 | 0.34519 | 0.55578 |
| C | 1.47903 | 0.14719 | -0.59080 |
| Br | 0.08932 | -1.24542 | -0.03009 |
| H | 4.36381 | 0.07347 | 1.33637 |
| H | 3.82531 | -1.17770 | -2.73497 |
| H | 1.43109 | -0.52415 | -2.65061 |
| H | 0.75861 | 0.98327 | -0.74461 |
| Br | -3.05527 | -0.93808 | 0.46480 |
| H | -2.35865 | 0.43664 | -0.08707 |
| Br | -1.44282 | 1.92383 | -0.71906 |
| H | 5.23652 | -0.87799 | -0.73074 |
| O | 1.80461 | 0.92861 | 1.58238 |
| C | 2.53003 | 1.15132 | 2.80173 |
| H | 1.82000 | 1.62482 | 3.47016 |
| H | 2.86468 | 0.20317 | 3.22143 |
| H | 3.37708 | 1.81359 | 2.62496 |

**Direct *para*-substitution TS**

| | | | |
|---|---|---|---|
| C | 2.59741 | 1.03877 | 0.95356 |
| C | 3.46310 | -0.39965 | -0.86673 |
| C | 3.64017 | 0.27235 | 0.36777 |
| C | 2.26483 | -0.30770 | -1.49555 |
| C | 1.40027 | 1.11569 | 0.33953 |
| C | 1.14407 | 0.41097 | -0.91427 |
| Br | -0.12382 | -1.06704 | -0.41362 |
| H | 2.79450 | 1.53036 | 1.89440 |
| H | 4.26281 | -0.97906 | -1.29883 |
| H | 2.10726 | -0.79740 | -2.44661 |
| H | 0.52382 | 0.98349 | -1.60225 |
| Br | -3.14061 | -1.24224 | 0.51453 |
| H | -2.67165 | 0.33598 | 0.21353 |
| Br | -2.06217 | 1.95648 | -0.13613 |
| H | 0.56292 | 1.67364 | 0.74598 |
| O | 4.75078 | 0.23813 | 1.05158 |
| C | 5.88052 | -0.50668 | 0.58799 |
| H | 6.64474 | -0.36773 | 1.34400 |
| H | 5.62998 | -1.56309 | 0.50340 |
| H | 6.22825 | -0.11557 | -0.36708 |

**Direct *meta*-substitution TS**

| | | | |
|---|---|---|---|
| C | -3.45946 | -0.01443 | -0.29059 |
| C | -2.58490 | 1.06704 | 1.72640 |
| C | -3.63468 | 0.47216 | 1.00201 |
| C | -1.34848 | 1.18204 | 1.17618 |
| C | -2.21256 | 0.11641 | -0.88023 |
| C | -1.11039 | 0.70054 | -0.16708 |
| Br | 0.01759 | -0.97275 | 0.04380 |
| H | -2.77732 | 1.42351 | 2.72763 |
| H | -4.60047 | 0.38643 | 1.47965 |
| H | -0.50792 | 1.62719 | 1.69110 |
| H | -2.06029 | -0.22828 | -1.89338 |
| H | -0.36219 | 1.30008 | -0.71825 |
| Br | 3.14792 | -1.33740 | 0.16849 |
| H | 2.71810 | 0.16897 | -0.09289 |
| Br | 2.01553 | 1.90957 | -0.39445 |
| O | -4.41017 | -0.60533 | -1.03127 |
| C | -5.70487 | -0.75668 | -0.48148 |
| H | -6.29371 | -1.25885 | -1.24201 |
| H | -5.68270 | -1.37175 | 0.42127 |
| H | -6.15656 | 0.21307 | -0.25882 |

**2,3-*ortho*-addition TS1**

| | | | |
|---|---|---|---|
| C | 2.89809 | -0.02805 | -0.07795 |
| C | 2.45407 | 1.99088 | 1.10635 |
| C | 3.17166 | 0.80727 | 0.98632 |
| C | 1.45054 | 2.39242 | 0.21587 |
| C | 1.77350 | 0.27083 | -0.98875 |
| C | 1.11558 | 1.57672 | -0.81577 |
| H | 2.69518 | 2.64378 | 1.93591 |
| H | 3.94055 | 0.57045 | 1.70364 |
| H | 0.91048 | 3.31262 | 0.37338 |
| H | 2.00680 | 0.03224 | -2.02305 |
| H | 0.32758 | 1.84173 | -1.50603 |
| Br | -2.02623 | 1.84281 | -0.08903 |
| H | -2.49446 | -0.07270 | 0.20890 |
| Br | 0.35237 | -1.02427 | -0.47594 |
| Br | -2.74841 | -1.57909 | 0.41258 |
| O | 3.55209 | -1.11545 | -0.38156 |
| C | 4.56141 | -1.60471 | 0.50273 |
| H | 4.13097 | -1.80902 | 1.48236 |
| H | 4.92101 | -2.52356 | 0.05440 |
| H | 5.37560 | -0.88495 | 0.58374 |

**2,3-*meta*-addition TS1**

| | | | |
|---|---|---|---|
| C | -1.65355 | 2.57590 | 0.34861 |
| C | -3.00996 | 0.68871 | 0.93263 |
| C | -2.51763 | 1.97831 | 1.20658 |
| C | -2.65393 | -0.02323 | -0.21123 |
| C | -1.16331 | 1.84617 | -0.80947 |
| C | -1.71257 | 0.52521 | -1.06128 |
| H | -1.26940 | 3.56960 | 0.52457 |
| H | -3.70031 | 0.24285 | 1.63538 |
| H | -2.84312 | 2.48357 | 2.10374 |
| H | -1.04311 | 2.44048 | -1.71246 |
| Br | 0.12592 | -1.92940 | -0.15862 |
| H | 1.83662 | -1.12213 | 0.15002 |
| Br | 0.79090 | 1.53245 | -0.30874 |
| Br | 3.15766 | -0.28862 | 0.35880 |
| H | -1.41120 | -0.01988 | -1.94304 |
| O | -3.17151 | -1.20430 | -0.55491 |
| C | -3.58198 | -2.08713 | 0.47980 |
| H | -3.73194 | -3.05012 | 0.00319 |
| H | -2.79444 | -2.17821 | 1.22978 |
| H | -4.52048 | -1.76062 | 0.93410 |

**2,3-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | 2.84617 | -0.83732 | -0.27646 |
| C | 2.86627 | 1.57452 | -0.55651 |
| C | 3.51637 | 0.31509 | -0.25084 |
| C | 1.52838 | 1.67229 | -0.58474 |
| C | 1.42718 | -0.79377 | -0.73749 |
| C | 0.68704 | 0.46369 | -0.31249 |
| H | 3.30749 | -1.78904 | -0.06451 |
| H | 3.45443 | 2.47086 | -0.69018 |
| H | 4.56938 | 0.32842 | -0.00542 |
| H | 1.42151 | -0.75547 | -1.83217 |
| H | -0.27810 | 0.49689 | -0.80550 |
| Br | 0.21370 | 0.49342 | 1.62340 |
| H | -2.22881 | -0.04333 | 0.71643 |
| Br | 0.43994 | -2.42066 | -0.33390 |
| Br | -3.23842 | 0.06678 | -0.28782 |
| O | 0.95500 | 2.88359 | -0.71406 |
| C | -0.40024 | 2.97953 | -1.11451 |
| H | -0.57458 | 2.45974 | -2.05981 |
| H | -1.08031 | 2.59609 | -0.35213 |
| H | -0.59059 | 4.03937 | -1.25488 |

**2,3-*ortho*-addition I1**

| | | | |
|---|---|---|---|
| C | 2.26053 | 0.93892 | -0.33056 |
| C | 0.51971 | 2.55887 | -0.76725 |
| C | 1.86965 | 2.22521 | -0.35633 |
| C | -0.44511 | 1.63944 | -0.86224 |
| C | 1.30204 | -0.10236 | -0.85481 |
| C | -0.14327 | 0.22511 | -0.52766 |
| H | 0.29350 | 3.59814 | -0.96408 |
| H | 2.54429 | 3.02248 | -0.08681 |
| H | -1.46638 | 1.89795 | -1.10098 |
| H | 1.36051 | -0.06194 | -1.94637 |
| H | -0.80525 | -0.47801 | -1.02031 |
| Br | -0.55451 | -0.06617 | 1.41554 |
| H | -2.97800 | -0.04998 | 0.57039 |
| Br | 1.78368 | -1.93023 | -0.42936 |
| Br | -4.06719 | -0.00106 | -0.35646 |
| O | 3.45886 | 0.47224 | 0.01277 |
| C | 4.41839 | 1.40224 | 0.47109 |
| H | 4.05104 | 1.93308 | 1.35195 |
| H | 5.29931 | 0.82393 | 0.73129 |
| H | 4.66921 | 2.12289 | -0.31074 |

**2,3-*ortho*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -2.69116 | -0.83934 | 0.11145 |
| C | -1.16636 | -1.56312 | 1.79350 |
| C | -2.47748 | -1.40225 | 1.34811 |
| C | -0.03343 | -1.19877 | 1.05638 |
| C | -1.54427 | -0.32704 | -0.68522 |
| C | -0.19835 | -0.59902 | -0.14770 |
| H | -1.02027 | -2.01157 | 2.76856 |
| H | 0.96542 | -1.37744 | 1.42512 |
| H | -1.63205 | -0.63094 | -1.72723 |
| H | 0.65900 | -0.30872 | -0.74139 |
| Br | 2.34906 | 1.48438 | 0.83906 |
| H | 2.74780 | 0.11108 | 0.08188 |
| Br | -1.69981 | 1.63244 | -0.71080 |
| Br | 2.98692 | -1.48189 | -0.78393 |
| H | -3.29773 | -1.73709 | 1.96243 |
| C | -5.04143 | -1.09042 | 0.19234 |
| H | -5.84808 | -0.85974 | -0.49373 |
| H | -5.02492 | -2.15872 | 0.40574 |
| H | -5.15691 | -0.51750 | 1.11167 |
| O | -3.84297 | -0.70155 | -0.48221 |

**2,3-*meta*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | 2.01844 | -2.12243 | -0.52700 |
| C | 3.30522 | -0.10033 | -0.53308 |
| C | 3.22384 | -1.50996 | -0.52045 |
| C | 2.18047 | 0.72248 | -0.56819 |
| C | 0.78986 | -1.32366 | -0.52813 |
| C | 0.93253 | 0.12699 | -0.61736 |
| H | 4.28931 | 0.34801 | -0.53786 |
| H | -0.01188 | -1.66661 | -1.18929 |
| H | 0.04708 | 0.73047 | -0.75984 |
| Br | -1.37177 | 1.76423 | 1.06418 |
| H | -2.04741 | 0.67717 | -0.18277 |
| Br | 0.05761 | -1.72381 | 1.27428 |
| Br | -2.47767 | -0.35675 | -1.39718 |
| H | 4.13803 | -2.08416 | -0.49477 |
| H | 1.92045 | -3.19697 | -0.48300 |
| O | 2.20995 | 2.05530 | -0.62035 |
| C | 3.45254 | 2.72078 | -0.51663 |
| H | 3.22188 | 3.78063 | -0.52845 |
| H | 3.95565 | 2.47327 | 0.42142 |
| H | 4.10369 | 2.48430 | -1.36245 |

**2,3-*meta*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -2.44117 | -0.42364 | 1.60438 |
| C | -0.71238 | 1.29954 | 1.58625 |
| C | -1.74679 | 0.52140 | 2.24183 |
| C | -0.26055 | 0.92347 | 0.38060 |
| C | -2.18125 | -0.69143 | 0.17088 |
| C | -0.78536 | -0.30421 | -0.27829 |
| H | -3.23400 | -0.97271 | 2.08962 |
| H | -0.30683 | 2.16004 | 2.09480 |
| H | -2.40219 | -1.71202 | -0.11667 |
| Br | 4.06827 | 0.15713 | -0.33464 |
| H | 2.69529 | -0.22820 | -0.32771 |
| Br | -3.46730 | 0.36903 | -0.93482 |
| Br | 0.45065 | -1.80244 | 0.15321 |
| H | -1.95983 | 0.73800 | 3.27964 |
| H | -0.71781 | -0.22233 | -1.35627 |
| O | 0.69897 | 1.50735 | -0.35032 |
| C | 1.31072 | 2.66833 | 0.17915 |
| H | 1.80874 | 2.44809 | 1.12579 |
| H | 2.04835 | 2.98153 | -0.55236 |
| H | 0.57055 | 3.45790 | 0.32579 |

**2,3-*ortho*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -2.29877 | -0.62911 | 0.31020 |
| C | -0.76557 | -0.47883 | 2.16977 |
| C | -2.01670 | -0.92516 | 1.58888 |
| C | 0.23253 | 0.01236 | 1.43095 |
| C | -1.35680 | 0.18976 | -0.50498 |
| C | 0.08213 | 0.09779 | -0.03718 |
| H | -0.64366 | -0.57379 | 3.24013 |
| H | 1.17439 | 0.31183 | 1.86575 |
| H | -1.45516 | -0.04336 | -1.55817 |
| H | 0.68600 | 0.87701 | -0.48650 |
| Br | 4.05086 | 0.47962 | 0.25447 |
| H | 3.12033 | -0.48284 | -0.24522 |
| Br | -1.92014 | 2.08604 | -0.38625 |
| Br | 0.85112 | -1.57336 | -0.86899 |
| H | -2.71050 | -1.47349 | 2.20661 |
| O | -3.40222 | -0.94737 | -0.37606 |
| C | -4.41937 | -1.64801 | 0.30927 |
| H | -4.05387 | -2.61315 | 0.66782 |
| H | -4.79149 | -1.06317 | 1.15363 |
| H | -5.21728 | -1.80345 | -0.41001 |

**2,3-*ortho*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 0.74765 | 2.92661 | -0.54443 |
| C | 1.32692 | 1.94081 | -1.36288 |
| C | 1.32354 | 0.62121 | -0.93609 |
| C | 0.70799 | 0.20326 | 0.34551 |
| C | -0.01310 | 1.27486 | 1.06418 |
| C | 0.11413 | 2.60207 | 0.65611 |
| Br | 1.99986 | -0.64188 | 1.52783 |
| H | 0.80210 | 3.97422 | -0.86152 |
| H | -0.04878 | -0.77130 | 0.08061 |
| H | -0.43785 | 1.01746 | 2.04644 |
| H | -0.35103 | 3.38946 | 1.25491 |
| Br | -1.33779 | -2.09196 | -0.40151 |
| Br | -2.41943 | 0.99424 | 0.14268 |
| H | -2.18051 | -0.65425 | -0.18745 |
| H | 1.77130 | 2.23005 | -2.31207 |
| O | 1.83516 | -0.43640 | -1.58276 |
| C | 2.40384 | -0.24646 | -2.91362 |
| H | 1.63880 | 0.13399 | -3.59782 |
| H | 3.28151 | 0.40279 | -2.85749 |
| H | 2.68459 | -1.27954 | -3.17137 |

**2,3-*meta*-elimination TS3**

| | | | |
|---|---|---|---|
| C | -2.18575 | -1.18096 | 1.40300 |
| C | -1.04263 | -1.53250 | 2.16630 |
| C | 0.18427 | -1.54464 | 1.60769 |
| C | 0.35606 | -1.09947 | 0.23068 |
| C | -0.82887 | -0.71863 | -0.50741 |
| C | -2.09275 | -0.78754 | 0.08480 |
| Br | 1.50080 | -2.27679 | -0.82274 |
| H | 1.06936 | -1.81047 | 2.16619 |
| H | 1.02730 | -0.16957 | 0.30918 |
| Br | 2.28244 | 1.55763 | 0.50169 |
| Br | -0.88658 | 2.16999 | -0.52529 |
| H | 0.74904 | 1.98052 | 0.00582 |
| H | -1.17700 | -1.80590 | 3.20270 |
| H | -3.15332 | -1.23280 | 1.88098 |
| H | -0.75044 | -0.51750 | -1.56424 |
| O | -3.12133 | -0.46689 | -0.70652 |
| C | -4.39129 | -0.27545 | -0.11477 |
| H | -5.04074 | 0.07821 | -0.90877 |
| H | -4.79131 | -1.21008 | 0.28662 |
| H | -4.33969 | 0.47862 | 0.67367 |

**3,4-met*a*-addition TS1**

| | | | |
|---|---|---|---|
| C | -2.70161 | -0.57137 | 0.63555 |
| C | -2.74055 | 1.52162 | -0.53949 |
| C | -3.25246 | 0.21203 | -0.32987 |
| C | -1.69831 | 2.04434 | 0.19094 |
| C | -1.56131 | -0.08708 | 1.39866 |
| C | -1.10790 | 1.27370 | 1.17022 |
| H | -3.04145 | -1.57639 | 0.83046 |
| H | -3.20619 | 2.10757 | -1.32160 |
| H | -1.31434 | 3.03055 | -0.01806 |
| H | -1.55433 | -0.38125 | 2.44478 |
| H | -0.30017 | 1.66547 | 1.76994 |
| Br | 1.72017 | 1.96082 | -0.18406 |
| H | 2.43881 | 0.19139 | -0.40688 |
| Br | 0.06442 | -1.11854 | 0.69967 |
| Br | 2.87718 | -1.31630 | -0.52072 |
| O | -4.26567 | -0.12301 | -1.14186 |
| C | -4.80405 | -1.42629 | -1.02114 |
| H | -4.03941 | -2.18387 | -1.20664 |
| H | -5.24255 | -1.57880 | -0.03188 |
| H | -5.57991 | -1.50171 | -1.77575 |

**3,4-*para*-addition TS1**

| | | | |
|---|---|---|---|
| C | 1.48888 | 1.70749 | -1.27390 |
| C | 2.63520 | 0.24019 | 0.22124 |
| C | 2.26905 | 0.62122 | -1.09965 |
| C | 2.26197 | 1.03985 | 1.34235 |
| C | 0.92612 | 2.44397 | -0.15053 |
| C | 1.46076 | 2.10399 | 1.16341 |
| H | 1.19162 | 2.00678 | -2.26942 |
| H | 2.58470 | 0.03143 | -1.94404 |
| H | 2.60445 | 0.72937 | 2.31746 |
| H | 0.75097 | 3.49910 | -0.32421 |
| H | 1.13568 | 2.69459 | 2.00853 |
| Br | 0.12293 | -2.01257 | 0.07629 |
| H | -1.48138 | -1.31858 | 0.04160 |
| Br | -0.96069 | 1.61780 | -0.09412 |
| Br | -2.98120 | -0.57270 | 0.02430 |
| O | 3.37787 | -0.78228 | 0.49836 |
| C | 3.70535 | -1.74825 | -0.51075 |
| H | 2.78467 | -2.13241 | -0.94869 |
| H | 4.35707 | -1.30211 | -1.26094 |
| H | 4.22859 | -2.53920 | 0.01373 |

**3,4-*para*-addition I1**

| | | | |
|---|---|---|---|
| C | -2.06240 | 1.48098 | 0.15724 |
| C | -2.91669 | -0.68376 | -0.51059 |
| C | -3.08016 | 0.62347 | 0.12563 |
| C | -1.68983 | -1.15556 | -0.78794 |
| C | -0.78837 | 1.11597 | -0.53397 |
| C | -0.48845 | -0.36842 | -0.44038 |
| H | -2.15013 | 2.44924 | 0.62664 |
| H | -4.02041 | 0.88327 | 0.58783 |
| H | -1.56806 | -2.15714 | -1.17232 |
| H | -0.91321 | 1.31058 | -1.60337 |
| H | 0.36756 | -0.62184 | -1.05569 |
| Br | 0.14233 | -0.89988 | 1.40239 |
| H | 2.50808 | -0.90055 | 0.37268 |
| Br | 0.69360 | 2.26406 | -0.02320 |
| Br | 3.51834 | -0.99501 | -0.63529 |
| O | -3.97969 | -1.46622 | -0.78500 |
| C | -5.28659 | -0.95189 | -0.62951 |
| H | -5.53594 | -0.80002 | 0.42293 |
| H | -5.42094 | -0.01609 | -1.17601 |
| H | -5.95347 | -1.70346 | -1.04191 |

**3,4-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | -0.07533 | 1.18046 | 1.02243 |
| C | 0.62452 | 2.77197 | -0.68025 |
| C | -0.36195 | 2.24572 | 0.26110 |
| C | 1.69842 | 2.06135 | -1.01745 |
| C | 1.30914 | 0.61904 | 0.94289 |
| C | 1.92313 | 0.70272 | -0.44368 |
| H | -0.76171 | 0.77009 | 1.74434 |
| H | 0.42195 | 3.73556 | -1.12600 |
| H | 2.39411 | 2.41435 | -1.76522 |
| H | 1.97792 | 1.20417 | 1.58097 |
| H | 2.97325 | 0.43576 | -0.40830 |
| Br | 1.17015 | -0.61219 | -1.73319 |
| H | -1.25994 | -1.01326 | -0.64581 |
| Br | 1.41496 | -1.16615 | 1.71822 |
| Br | -2.60480 | -1.38727 | -0.34453 |
| O | -1.51245 | 2.93932 | 0.24829 |
| C | -2.53893 | 2.50465 | 1.11716 |
| H | -2.82744 | 1.47496 | 0.89597 |
| H | -2.22155 | 2.57779 | 2.16081 |
| H | -3.38191 | 3.16718 | 0.94622 |

**3,4-*para*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | 2.91848 | 0.05725 | -0.87532 |
| C | 1.69462 | 1.83197 | 0.17595 |
| C | 2.93439 | 1.25387 | -0.27336 |
| C | 0.46039 | 1.18172 | -0.01767 |
| C | 1.66253 | -0.68800 | -1.08407 |
| C | 0.43424 | -0.03136 | -0.60521 |
| H | 3.83429 | -0.39937 | -1.22445 |
| H | -0.45606 | 1.65215 | 0.30850 |
| H | 1.54678 | -0.95845 | -2.13580 |
| H | -0.51335 | -0.53107 | -0.75626 |
| Br | -2.10192 | -0.67868 | 1.65989 |
| H | -2.50856 | 0.00585 | 0.23702 |
| Br | 1.84053 | -2.41338 | -0.16318 |
| Br | -2.75590 | 0.76688 | -1.38866 |
| H | 3.86558 | 1.77668 | -0.12263 |
| O | 1.63753 | 2.97912 | 0.77839 |
| C | 2.81106 | 3.75095 | 1.05870 |
| H | 3.47974 | 3.19635 | 1.71455 |
| H | 3.31270 | 4.02820 | 0.13312 |
| H | 2.44980 | 4.63945 | 1.56311 |

**3,4-met*a*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -2.69041 | -0.35080 | -0.53313 |
| C | -1.45681 | -1.71802 | 1.01844 |
| C | -2.69586 | -1.29313 | 0.43558 |
| C | -0.23548 | -1.21815 | 0.64486 |
| C | -1.41354 | 0.22677 | -0.97723 |
| C | -0.18402 | -0.24916 | -0.33709 |
| H | -3.59153 | 0.01118 | -1.00254 |
| H | -1.52194 | -2.47209 | 1.79284 |
| H | 0.68159 | -1.55816 | 1.09990 |
| H | -1.29113 | 0.14019 | -2.06079 |
| H | 0.75749 | 0.15685 | -0.67067 |
| Br | 2.33728 | 0.96957 | 1.35753 |
| H | 2.70324 | -0.21822 | 0.20204 |
| Br | -1.42923 | 2.17987 | -0.68416 |
| Br | 2.83015 | -1.42622 | -1.02383 |
| O | -3.76820 | -1.90788 | 0.94859 |
| C | -5.04200 | -1.52762 | 0.46052 |
| H | -5.22579 | -0.46627 | 0.64131 |
| H | -5.13128 | -1.74049 | -0.60728 |
| H | -5.76359 | -2.12193 | 1.01084 |

**3,4-*para*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | 0.14576 | 1.47507 | -0.06136 |
| C | -0.26756 | 1.25974 | 1.32098 |
| C | -1.18258 | 0.34547 | 1.62833 |
| C | -1.81738 | -0.47440 | 0.56517 |
| C | -0.97983 | -0.58809 | -0.69500 |
| C | -0.19212 | 0.60812 | -1.03219 |
| Br | -3.55112 | 0.37515 | 0.07852 |
| H | -1.51783 | 0.20336 | 2.64544 |
| H | -2.11895 | -1.45141 | 0.92144 |
| H | -1.57704 | -0.94431 | -1.52471 |
| H | 0.14115 | 0.72127 | -2.05099 |
| Br | 3.52186 | 0.02542 | 0.43156 |
| Br | 0.26300 | -2.17463 | -0.41063 |
| H | 2.35403 | -0.74805 | 0.14425 |
| H | 0.18680 | 1.88861 | 2.07303 |
| O | 0.87596 | 2.58636 | -0.20971 |
| C | 1.40814 | 2.85830 | -1.48990 |
| H | 2.08407 | 2.05955 | -1.80365 |
| H | 0.61172 | 2.97933 | -2.22811 |
| H | 1.96079 | 3.78783 | -1.39592 |

**3,4-met*a*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | 2.39683 | -0.31115 | 0.38121 |
| C | 1.18120 | -0.95094 | -1.63731 |
| C | 2.35972 | -0.98719 | -0.77834 |
| C | 0.03093 | -0.44391 | -1.20361 |
| C | 1.24382 | 0.52132 | 0.77666 |
| C | -0.08093 | 0.09449 | 0.17402 |
| H | 3.27029 | -0.28931 | 1.01270 |
| H | 1.27943 | -1.37495 | -2.62649 |
| H | -0.85666 | -0.44055 | -1.82022 |
| H | 1.15796 | 0.62835 | 1.85070 |
| H | -0.82270 | 0.87976 | 0.25465 |
| Br | -3.90831 | 0.18752 | -0.68498 |
| H | -3.09952 | -0.61867 | 0.17208 |
| Br | 1.54783 | 2.42639 | 0.19776 |
| Br | -0.84885 | -1.34851 | 1.33587 |
| O | 3.34442 | -1.74151 | -1.29189 |
| C | 4.54546 | -1.84103 | -0.55725 |
| H | 5.00823 | -0.85983 | -0.42731 |
| H | 4.36860 | -2.29164 | 0.42243 |
| H | 5.20350 | -2.47976 | -1.13842 |

**3,4-met*a*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 1.80289 | -2.11563 | -0.78516 |
| C | 2.25393 | -1.32344 | 0.31074 |
| C | 1.76621 | -0.06853 | 0.46979 |
| C | 0.72269 | 0.42835 | -0.42003 |
| C | 0.27687 | -0.43111 | -1.49566 |
| C | 0.84053 | -1.68829 | -1.65968 |
| Br | 1.09734 | 2.22855 | -1.08800 |
| H | 2.07232 | 0.57943 | 1.27604 |
| H | -0.18340 | 0.63965 | 0.25004 |
| H | -0.41686 | -0.03227 | -2.21811 |
| H | 0.50884 | -2.32626 | -2.46434 |
| Br | -1.80794 | 1.00633 | 1.60427 |
| Br | -2.33801 | -1.47853 | -0.64155 |
| H | -2.16895 | -0.24589 | 0.54000 |
| H | 2.25417 | -3.09237 | -0.90169 |
| O | 3.16652 | -1.92806 | 1.08644 |
| C | 3.65738 | -1.20937 | 2.20258 |
| H | 4.35775 | -1.87078 | 2.70202 |
| H | 4.17491 | -0.30083 | 1.88573 |
| H | 2.84731 | -0.95044 | 2.88799 |

**3,4-*para*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 2.57527 | 0.39641 | 0.56810 |
| C | 1.76711 | 0.94906 | 1.63514 |
| C | 0.46664 | 1.24073 | 1.39616 |
| C | -0.16255 | 0.96331 | 0.09081 |
| C | 0.69426 | 0.34129 | -0.93904 |
| C | 2.05149 | 0.15170 | -0.70733 |
| Br | -1.00330 | 2.57135 | -0.62699 |
| H | -0.17854 | 1.67475 | 2.17069 |
| H | -1.15721 | 0.24628 | 0.32723 |
| H | 0.27058 | 0.21959 | -1.94826 |
| H | 2.67251 | -0.25833 | -1.50489 |
| Br | -2.59912 | -0.98414 | 0.71273 |
| Br | 0.13730 | -2.23364 | -0.69290 |
| H | -1.37264 | -1.89048 | 0.01901 |
| H | 2.24137 | 1.11111 | 2.60637 |
| O | 3.84092 | 0.18800 | 0.95757 |
| C | 4.77992 | -0.42532 | 0.02111 |
| H | 4.41400 | -1.41208 | -0.28502 |
| H | 4.94787 | 0.24096 | -0.82971 |
| H | 5.68118 | -0.51351 | 0.64523 |

**2,5-*ortho*-addition TS1**

| | | | |
|---|---|---|---|
| C | -1.35576 | 2.02929 | 1.38987 |
| C | -1.97703 | 1.50754 | -0.92561 |
| C | -1.38760 | 2.34015 | -0.00437 |
| C | -2.43391 | 0.26254 | -0.52161 |
| C | -1.77619 | 0.82586 | 1.80738 |
| C | -2.18500 | -0.20341 | 0.84730 |
| Br | -0.41815 | -1.22731 | 0.54675 |
| H | -0.95523 | 2.75322 | 2.08184 |
| H | -1.72441 | 0.53649 | 2.84710 |
| H | -2.88718 | -0.93513 | 1.22678 |
| Br | 2.49784 | -1.42970 | -0.12614 |
| H | 2.10730 | 0.17499 | -0.25352 |
| Br | 1.62440 | 1.87415 | -0.36453 |
| H | -1.01444 | 3.29916 | -0.33034 |
| H | -2.05363 | 1.77945 | -1.96670 |
| O | -3.02444 | -0.48011 | -1.42146 |
| C | -3.53610 | -1.77558 | -1.10233 |
| H | -3.94506 | -2.15824 | -2.03055 |
| H | -2.73717 | -2.42658 | -0.75214 |
| H | -4.32828 | -1.70061 | -0.35745 |

**2,5-*meta*-addition TS1**

| | | | |
|---|---|---|---|
| C | 1.84315 | 0.77585 | 1.82101 |
| C | 2.41232 | 0.33923 | -0.52783 |
| C | 2.33731 | -0.07391 | 0.82260 |
| C | 1.88398 | 1.55223 | -0.87130 |
| C | 1.29230 | 1.97337 | 1.48820 |
| C | 1.18751 | 2.35521 | 0.09831 |
| Br | -0.80605 | 1.63114 | -0.17058 |
| H | 1.85288 | 0.43690 | 2.84548 |
| H | 0.86302 | 2.62340 | 2.23655 |
| H | 1.08036 | 3.40944 | -0.12050 |
| Br | -2.87880 | -0.42181 | -0.34464 |
| H | -1.54314 | -1.21080 | 0.07069 |
| Br | 0.03313 | -2.01695 | 0.55740 |
| H | 2.75396 | -1.02415 | 1.11468 |
| H | 1.90225 | 1.86517 | -1.90534 |
| O | 2.96192 | -0.39352 | -1.50391 |
| C | 3.45230 | -1.69192 | -1.20312 |
| H | 3.81259 | -2.09364 | -2.14465 |
| H | 4.28375 | -1.64404 | -0.49543 |
| H | 2.65639 | -2.32792 | -0.81396 |

**2,5-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | -0.80949 | 1.33474 | 0.68521 |
| C | -1.07787 | -1.44827 | 1.11743 |
| C | -2.02193 | 0.86292 | 0.98263 |
| C | 0.12703 | -0.97935 | 0.83027 |
| C | 0.36367 | 0.44101 | 0.47735 |
| C | -2.28421 | -0.58467 | 1.13199 |
| H | -1.22018 | -2.49454 | 1.34987 |
| H | -2.85961 | 1.52736 | 1.12939 |
| H | 0.99124 | -1.62958 | 0.82986 |
| H | -2.89568 | -0.78554 | 2.00743 |
| Br | -3.50268 | -1.21000 | -0.33604 |
| H | 1.24106 | 0.84922 | 0.97249 |
| O | -0.46642 | 2.62556 | 0.55667 |
| C | -1.48982 | 3.59290 | 0.64832 |
| H | -1.01353 | 4.55417 | 0.48246 |
| H | -2.25396 | 3.42448 | -0.11403 |
| H | -1.95460 | 3.58193 | 1.63740 |
| Br | 0.89493 | 0.52289 | -1.44863 |
| H | 3.19220 | -0.27168 | -0.54424 |
| Br | 4.14089 | -0.71506 | 0.42914 |

**2,5-*ortho*-addition I1**

| | | | |
|---|---|---|---|
| C | -0.00036 | 0.76595 | 1.57857 |
| C | 1.95970 | 1.93916 | -0.10333 |
| C | 1.10851 | 0.06651 | 1.31827 |
| C | 0.85851 | 2.63035 | 0.14914 |
| C | -0.26836 | 2.06312 | 0.92779 |
| C | 2.14295 | 0.53882 | 0.35315 |
| H | -0.73832 | 0.40698 | 2.27924 |
| H | 2.76526 | 2.37049 | -0.68124 |
| H | 0.74294 | 3.63935 | -0.22180 |
| H | 3.13306 | 0.36910 | 0.76758 |
| Br | 2.12557 | -0.63822 | -1.24441 |
| Br | -1.83991 | 1.88951 | -0.33795 |
| Br | -1.84182 | -2.17411 | -0.40133 |
| H | -1.68995 | -0.75748 | -0.50054 |
| H | -0.66949 | 2.78744 | 1.63049 |
| O | 1.46353 | -1.09454 | 1.87973 |
| C | 0.56211 | -1.69801 | 2.78652 |
| H | -0.39609 | -1.89910 | 2.30409 |
| H | 1.02218 | -2.63330 | 3.08931 |
| H | 0.40948 | -1.06408 | 3.66371 |

**2,5-*ortho*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -1.07351 | -0.32634 | -1.52462 |
| C | 0.25068 | 0.52783 | 0.27376 |
| C | 0.12675 | -0.20626 | -0.94562 |
| C | -0.81701 | 1.16669 | 0.88351 |
| C | -2.28495 | 0.28186 | -0.93006 |
| C | -2.05915 | 1.10426 | 0.29394 |
| H | -1.21307 | -0.88467 | -2.43930 |
| H | -0.65210 | 1.72354 | 1.79181 |
| H | -2.84830 | 0.86384 | -1.65782 |
| Br | 2.67278 | -1.60324 | 0.97964 |
| H | 3.11558 | -0.20244 | 0.07173 |
| Br | -3.50113 | -1.18292 | -0.42903 |
| Br | 3.31892 | 1.24079 | -0.79975 |
| H | 1.01791 | -0.65116 | -1.35905 |
| H | 1.22733 | 0.59581 | 0.72559 |
| O | -3.12392 | 1.73479 | 0.69382 |
| C | -3.07396 | 2.54212 | 1.87563 |
| H | -2.34415 | 3.34122 | 1.75355 |
| H | -4.06927 | 2.95656 | 1.98490 |
| H | -2.82575 | 1.92616 | 2.73866 |

**2,5-*meta*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | 1.69528 | 0.21078 | -1.46347 |
| C | -0.03899 | -0.41221 | 0.05139 |
| C | 0.40039 | 0.28036 | -1.09393 |
| C | 0.82387 | -1.19926 | 0.85702 |
| C | 2.64634 | -0.60784 | -0.69576 |
| C | 2.13380 | -1.28759 | 0.49883 |
| H | 2.07077 | 0.73146 | -2.33286 |
| H | 3.10287 | -1.34422 | -1.36544 |
| H | 2.81952 | -1.87996 | 1.08837 |
| Br | -2.33904 | 1.82321 | 0.72141 |
| H | -2.84117 | 0.48061 | -0.25925 |
| Br | 4.17300 | 0.52884 | -0.18088 |
| Br | -3.07166 | -0.92849 | -1.15995 |
| H | -0.32954 | 0.86023 | -1.63945 |
| H | -1.07890 | -0.32723 | 0.31298 |
| O | 0.40908 | -1.84903 | 1.94150 |
| C | -0.96177 | -1.72397 | 2.34112 |
| H | -1.63049 | -2.12140 | 1.57678 |
| H | -1.04684 | -2.31065 | 3.24915 |
| H | -1.21300 | -0.68280 | 2.54633 |

**2,5-*meta*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -1.26189 | -1.12004 | -1.10994 |
| C | 0.33888 | 0.34512 | 0.05945 |
| C | -0.02451 | -0.86873 | -0.71009 |
| C | -0.81475 | 1.21115 | 0.42995 |
| C | -2.40039 | -0.21965 | -0.80307 |
| C | -2.05879 | 0.96585 | 0.01426 |
| H | -1.48285 | -2.01606 | -1.67316 |
| H | -2.93988 | 0.05138 | -1.70770 |
| H | -2.87619 | 1.61237 | 0.29384 |
| Br | 3.77938 | -1.45401 | 0.62630 |
| H | 3.36919 | -0.30645 | -0.11874 |
| Br | -3.78648 | -1.29654 | 0.16360 |
| Br | 1.61803 | 1.41651 | -1.04377 |
| H | 0.78118 | -1.54991 | -0.94752 |
| H | 0.93585 | 0.11141 | 0.93785 |
| O | -0.42875 | 2.22721 | 1.21751 |
| C | -1.41038 | 3.15003 | 1.63677 |
| H | -0.89413 | 3.88228 | 2.24978 |
| H | -1.86836 | 3.64849 | 0.77904 |
| H | -2.18645 | 2.65775 | 2.22791 |

**2,5-*ortho*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -0.97781 | -0.97561 | -1.22959 |
| C | 0.44783 | 0.40871 | 0.21808 |
| C | 0.22469 | -0.68263 | -0.75844 |
| C | -0.76092 | 1.14844 | 0.63137 |
| C | -2.20826 | -0.26114 | -0.80745 |
| C | -1.97059 | 0.86414 | 0.14192 |
| H | -1.10868 | -1.78276 | -1.93695 |
| H | -2.79189 | 0.08426 | -1.65724 |
| Br | 4.04471 | -1.24037 | 0.51380 |
| H | 3.52751 | -0.01179 | -0.00480 |
| Br | -3.42274 | -1.58465 | 0.04161 |
| Br | 1.73656 | 1.72097 | -0.63132 |
| H | 1.09311 | -1.24235 | -1.07746 |
| H | 1.04267 | 0.07288 | 1.06395 |
| H | -0.61803 | 1.95978 | 1.32812 |
| O | -3.10532 | 1.52456 | 0.41222 |
| C | -3.04199 | 2.61226 | 1.30909 |
| H | -4.05163 | 3.00412 | 1.38321 |
| H | -2.70413 | 2.28517 | 2.29532 |
| H | -2.37258 | 3.39081 | 0.93525 |

**2,5-*ortho*-elimination TS3**

| | | | |
|---|---|---|---|
| C | -0.77355 | 1.19965 | 0.45984 |
| C | 1.11323 | 1.88083 | -0.89408 |
| C | 0.34699 | 2.00036 | 0.28245 |
| C | 0.60240 | 1.08949 | -1.99575 |
| C | -1.12804 | 0.16024 | -0.52121 |
| C | -0.48977 | 0.30260 | -1.83805 |
| H | 1.13662 | 1.13952 | -2.94713 |
| H | -0.53461 | -0.90301 | -0.02698 |
| H | -0.89865 | -0.29424 | -2.65966 |
| Br | 0.70517 | -2.08317 | 0.65709 |
| H | 1.88596 | -0.94171 | 0.25794 |
| Br | -2.98920 | -0.33988 | -0.59041 |
| Br | 2.90737 | 0.34319 | -0.19496 |
| H | 1.89156 | 2.62883 | -1.10520 |
| H | 0.66860 | 2.70522 | 1.04641 |
| C | -1.25927 | 2.05113 | 2.66556 |
| H | -1.28966 | 3.10574 | 2.37885 |
| H | -2.07563 | 1.80079 | 3.35919 |
| H | -0.28820 | 1.75451 | 3.07545 |
| O | -1.59806 | 1.21173 | 1.51980 |

**2,5-*meta*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 0.89266 | 1.24712 | -0.70362 |
| C | -0.82651 | 1.62363 | 0.91096 |
| C | -0.32035 | 1.79678 | -0.39732 |
| C | -0.08333 | 0.97400 | 1.91140 |
| C | 1.57243 | 0.39637 | 0.24892 |
| C | 1.11447 | 0.40933 | 1.62266 |
| H | 1.29138 | 1.34712 | -1.70273 |
| H | -0.50365 | 0.90175 | 2.90278 |
| H | 1.13055 | -0.63498 | -0.06097 |
| H | 1.68422 | -0.13177 | 2.36357 |
| Br | -0.19208 | -2.34427 | -0.54573 |
| H | -1.46791 | -1.44590 | -0.11386 |
| Br | 3.47552 | 0.22020 | -0.00361 |
| Br | -2.88060 | -0.40528 | 0.38991 |
| H | -1.75667 | 2.09116 | 1.18732 |
| O | -0.95247 | 2.47278 | -1.36141 |
| C | -2.22211 | 3.05190 | -1.08847 |
| H | -2.14022 | 3.83066 | -0.32618 |
| H | -2.54208 | 3.50255 | -2.02212 |
| H | -2.93938 | 2.28972 | -0.78373 |

## HBr-assisted bromination of nitrobenzene in gas phase

**nitrobenzene**

| | | | |
|---|---|---|---|
| C | -1.81092 | -1.20343 | 0.00002 |
| C | -0.42652 | -1.21138 | 0.00001 |
| C | 0.23991 | 0.00000 | -0.00001 |
| C | -0.42652 | 1.21138 | -0.00002 |
| C | -1.81091 | 1.20343 | -0.00002 |
| C | -2.50091 | 0.00000 | 0.00001 |
| H | -2.35018 | -2.14003 | 0.00004 |
| H | 0.13654 | -2.13166 | 0.00002 |
| H | 0.13654 | 2.13166 | -0.00004 |
| H | -2.35018 | 2.14003 | -0.00003 |
| H | -3.58234 | 0.00000 | 0.00001 |
| N | 1.71452 | 0.00000 | -0.00002 |
| O | 2.27645 | 1.07459 | 0.00002 |
| O | 2.27645 | -1.07459 | 0.00000 |

***m*-bromonitrobenzene**

| | | | |
|---|---|---|---|
| C | 0.56710 | 2.28092 | 0.00021 |
| C | 1.54968 | 0.12031 | -0.00002 |
| C | 1.70526 | 1.49273 | 0.00005 |
| C | 0.31024 | -0.49174 | 0.00002 |
| C | -0.69204 | 1.70158 | 0.00014 |
| C | -0.80934 | 0.31983 | -0.00013 |
| Br | -2.52643 | -0.47193 | -0.00005 |
| H | 0.66033 | 3.35745 | 0.00032 |
| H | 0.23689 | -1.56765 | -0.00012 |
| H | -1.57872 | 2.31856 | 0.00019 |
| H | 2.69552 | 1.92008 | -0.00010 |
| N | 2.75336 | -0.73421 | 0.00004 |
| O | 3.83082 | -0.17957 | -0.00052 |
| O | 2.58821 | -1.93455 | 0.00047 |

***o*-bromonitrobenzene**

| | | | |
|---|---|---|---|
| C | 2.23438 | 0.34133 | 0.03312 |
| C | 1.97087 | -2.03520 | 0.05688 |
| C | 2.79496 | -0.92063 | 0.05958 |
| C | 0.59526 | -1.88908 | 0.02511 |
| C | 0.85721 | 0.48267 | 0.03145 |
| C | 0.02057 | -0.62553 | 0.02052 |
| Br | -1.85755 | -0.50718 | -0.08471 |
| H | 2.84725 | 1.23038 | 0.01596 |
| H | 2.39875 | -3.02772 | 0.07077 |
| H | -0.04694 | -2.75710 | 0.00030 |
| H | 3.86923 | -1.03281 | 0.07734 |
| N | 0.34444 | 1.86231 | 0.05177 |
| O | 0.87699 | 2.65105 | -0.69987 |
| O | -0.54005 | 2.12156 | 0.83467 |

***p*-bromonitrobenzene**

| | | | |
|---|---|---|---|
| C | -1.09977 | -1.20940 | 0.00005 |
| C | -1.09977 | 1.20940 | -0.00005 |
| C | -1.76875 | 0.00000 | 0.00000 |
| C | 0.28339 | 1.20905 | -0.00006 |
| C | 0.28339 | -1.20905 | 0.00005 |
| C | 0.96243 | 0.00000 | 0.00000 |
| Br | 2.85183 | 0.00000 | 0.00000 |
| H | -1.65867 | -2.13224 | 0.00008 |
| H | -1.65868 | 2.13224 | -0.00008 |
| H | 0.82772 | 2.14147 | -0.00010 |
| H | 0.82772 | -2.14147 | 0.00011 |
| N | -3.24149 | 0.00000 | 0.00000 |
| O | -3.80172 | -1.07518 | -0.00013 |
| O | -3.80171 | 1.07518 | 0.00013 |

**Direct *meta*-substitution TS**

| | | | |
|---|---|---|---|
| C | 2.38368 | 1.22869 | 1.89919 |
| C | 3.28015 | 0.09306 | -0.04222 |
| C | 3.45119 | 0.62647 | 1.22775 |
| C | 2.07280 | 0.13905 | -0.68656 |
| C | 1.15892 | 1.28681 | 1.29627 |
| C | 0.94849 | 0.74080 | -0.02425 |
| Br | -0.20697 | -0.90790 | 0.26939 |
| H | 2.53460 | 1.63676 | 2.88704 |
| H | 1.95740 | -0.27202 | -1.67893 |
| H | 0.29923 | 1.74205 | 1.77141 |
| H | 0.18865 | 1.30368 | -0.61549 |
| Br | -3.25276 | -1.34953 | 0.15548 |
| H | -2.84732 | 0.13649 | -0.19619 |
| Br | -2.11584 | 1.87217 | -0.58395 |
| H | 4.42715 | 0.55448 | 1.68743 |
| N | 4.43300 | -0.54575 | -0.71067 |
| O | 4.23928 | -1.01561 | -1.80647 |
| O | 5.48358 | -0.54514 | -0.11031 |

**2,3-*ortho*-addition TS1**

| | | | |
|---|---|---|---|
| C | 2.66104 | 0.18752 | 0.07778 |
| C | 2.12068 | 2.28973 | 1.04891 |
| C | 2.87152 | 1.08867 | 1.05859 |
| C | 1.18423 | 2.56268 | 0.07756 |
| C | 1.63399 | 0.35697 | -0.92846 |
| C | 0.93408 | 1.62943 | -0.91464 |
| H | 2.30706 | 3.01804 | 1.82617 |
| H | 3.61240 | 0.89836 | 1.81967 |
| H | 0.62466 | 3.48481 | 0.08997 |
| H | 1.86437 | -0.04919 | -1.90733 |
| H | 0.24385 | 1.84761 | -1.71427 |
| Br | -2.04917 | 1.79505 | -0.12667 |
| H | -2.52918 | -0.10257 | 0.19785 |
| Br | 0.12808 | -0.93890 | -0.33618 |
| Br | -2.65782 | -1.63329 | 0.39587 |
| N | 3.50264 | -1.02206 | 0.00437 |
| O | 3.47650 | -1.63689 | -1.03853 |
| O | 4.17189 | -1.29219 | 0.97396 |

**Direct para-substitution TS**

| | | | |
|---|---|---|---|
| C | 2.93426 | 0.19828 | 1.22778 |
| C | 2.93420 | 0.19843 | -1.22776 |
| C | 3.57086 | 0.07553 | -0.00001 |
| C | 1.58876 | 0.46371 | -1.22844 |
| C | 1.58881 | 0.46357 | 1.22855 |
| C | 0.86150 | 0.61478 | 0.00008 |
| Br | -0.43527 | -0.97301 | 0.00004 |
| H | 3.49815 | 0.07710 | 2.13889 |
| H | 3.49806 | 0.07736 | -2.13891 |
| H | 1.04193 | 0.56776 | -2.15524 |
| H | 0.02372 | 1.37168 | 0.00013 |
| Br | -3.44014 | -1.25500 | -0.00006 |
| H | -2.97407 | 0.26596 | -0.00002 |
| Br | -2.16161 | 1.99214 | 0.00002 |
| H | 1.04202 | 0.56750 | 2.15539 |
| N | 5.03107 | -0.21923 | -0.00006 |
| O | 5.56741 | -0.32647 | 1.07759 |
| O | 5.56735 | -0.32639 | -1.07774 |

**2,3-*meta*-addition TS1**

| | | | |
|---|---|---|---|
| C | -1.29235 | 2.71067 | -0.06342 |
| C | -2.75863 | 1.18202 | 1.03480 |
| C | -2.14475 | 2.43918 | 0.96451 |
| C | -2.52170 | 0.21937 | 0.07141 |
| C | -0.90879 | 1.67597 | -1.01138 |
| C | -1.60796 | 0.39403 | -0.93710 |
| H | -0.84270 | 3.68609 | -0.17891 |
| H | -3.46378 | 0.95251 | 1.82126 |
| H | -2.37325 | 3.18825 | 1.70687 |
| H | -0.71904 | 2.00952 | -2.02622 |
| H | -1.52502 | -0.32206 | -1.73705 |
| Br | 0.16949 | -1.86986 | -0.17728 |
| H | 1.92263 | -1.17300 | 0.18744 |
| Br | 1.01344 | 1.40668 | -0.33523 |
| Br | 3.25420 | -0.36883 | 0.42787 |
| N | -3.30783 | -1.02855 | 0.11423 |
| O | -3.33477 | -1.68930 | -0.89544 |
| O | -3.88252 | -1.27926 | 1.15002 |

**2,3-*ortho*-addition I1**

| | | | |
|---|---|---|---|
| C | 2.10076 | 1.00223 | -0.26909 |
| C | 0.34407 | 2.64416 | -0.49963 |
| C | 1.70453 | 2.26905 | -0.15924 |
| C | -0.59495 | 1.71146 | -0.65856 |
| C | 1.17405 | -0.05557 | -0.78872 |
| C | -0.27536 | 0.27317 | -0.43709 |
| H | 0.10726 | 3.69328 | -0.59969 |
| H | 2.41993 | 3.02282 | 0.13608 |
| H | -1.62528 | 1.96577 | -0.86429 |
| H | 1.23486 | -0.05792 | -1.87977 |
| H | -0.93867 | -0.38576 | -0.98616 |
| Br | -0.72550 | -0.10168 | 1.46417 |
| H | -3.20626 | -0.17410 | 0.53558 |
| Br | 1.62465 | -1.88054 | -0.29682 |
| Br | -4.17438 | -0.03008 | -0.50384 |
| N | 3.53147 | 0.72816 | -0.13664 |
| O | 4.01150 | -0.02102 | -0.96062 |
| O | 4.13878 | 1.29630 | 0.74383 |

**2,3-*ortho*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -2.43072 | -0.82457 | 0.34079 |
| C | -0.83109 | -1.34331 | 2.03605 |
| C | -2.18133 | -1.31806 | 1.55860 |
| C | 0.22507 | -0.89856 | 1.28733 |
| C | -1.37554 | -0.26932 | -0.51439 |
| C | -0.01163 | -0.38753 | 0.01568 |
| H | -0.65013 | -1.74961 | 3.02195 |
| H | 1.23953 | -0.93445 | 1.65149 |
| H | -1.46068 | -0.56936 | -1.55633 |
| H | 0.79837 | -0.05537 | -0.61156 |
| Br | 2.52554 | 1.48168 | 0.62937 |
| H | 2.86981 | -0.10820 | -0.10594 |
| Br | -1.56959 | 1.70513 | -0.56285 |
| Br | 2.90939 | -1.60877 | -0.77995 |
| H | -2.98905 | -1.70376 | 2.16240 |
| N | -3.79947 | -0.85265 | -0.20004 |
| O | -3.91124 | -0.63292 | -1.38604 |
| O | -4.69709 | -1.10382 | 0.56902 |

**2,3-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | -2.12271 | 1.97569 | -0.26996 |
| C | -3.17781 | -0.19133 | -0.39022 |
| C | -3.22563 | 1.23764 | -0.14057 |
| C | -2.00095 | -0.81438 | -0.46338 |
| C | -0.85851 | 1.32493 | -0.74020 |
| C | -0.70865 | -0.10900 | -0.25242 |
| H | -4.08827 | -0.76281 | -0.49370 |
| H | -0.90236 | 1.25666 | -1.83168 |
| H | 0.11253 | -0.60794 | -0.75352 |
| Br | -0.24797 | -0.23529 | 1.66999 |
| H | 2.20670 | -0.90071 | 0.70981 |
| Br | 0.70718 | 2.41969 | -0.40501 |
| Br | 3.14406 | -1.13625 | -0.33734 |
| H | -4.16952 | 1.68934 | 0.12664 |
| H | -2.13038 | 3.04480 | -0.11703 |
| N | -1.95500 | -2.26599 | -0.66497 |
| O | -0.85523 | -2.77715 | -0.70872 |
| O | -3.00634 | -2.85835 | -0.78035 |

**2,3-*meta*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | 1.62380 | 2.31088 | 0.63012 |
| C | 3.21625 | 0.55656 | 0.41389 |
| C | 2.92678 | 1.91816 | 0.50963 |
| C | 2.21238 | -0.40808 | 0.48820 |
| C | 0.52939 | 1.34006 | 0.60634 |
| C | 0.89864 | -0.08040 | 0.61307 |
| H | 4.23782 | 0.21519 | 0.30967 |
| H | -0.33582 | 1.51591 | 1.25950 |
| H | 0.13120 | -0.82628 | 0.76569 |
| Br | -1.28065 | -1.65920 | -1.22400 |
| H | -1.98552 | -0.79142 | 0.06446 |
| Br | -0.16926 | 1.82501 | -1.18446 |
| Br | -2.49839 | 0.13415 | 1.42565 |
| H | 3.72505 | 2.64348 | 0.48211 |
| H | 1.35727 | 3.35516 | 0.71050 |
| N | 2.61404 | -1.83270 | 0.48804 |
| O | 1.80741 | -2.62685 | 0.89310 |
| O | 3.73244 | -2.07378 | 0.08473 |

**2,3-*ortho*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -2.17687 | -0.48177 | 0.44897 |
| C | -0.64092 | -0.46160 | 2.30603 |
| C | -1.93036 | -0.77703 | 1.72495 |
| C | 0.38576 | -0.10789 | 1.52997 |
| C | -1.19472 | 0.21811 | -0.40954 |
| C | 0.23095 | -0.02166 | 0.05436 |
| H | -0.51620 | -0.56020 | 3.37423 |
| H | 1.36792 | 0.07973 | 1.94013 |
| H | -1.32707 | -0.02137 | -1.45627 |
| H | 0.90337 | 0.70469 | -0.38690 |
| Br | 4.07288 | 0.49651 | 0.11006 |
| H | 3.31853 | -0.62915 | -0.33291 |
| Br | -1.53707 | 2.16860 | -0.32285 |
| Br | 0.85889 | -1.75016 | -0.71639 |
| H | -2.69884 | -1.25102 | 2.31734 |
| N | -3.47859 | -0.80754 | -0.13785 |
| O | -3.62429 | -0.56018 | -1.31763 |
| O | -4.32007 | -1.30256 | 0.58043 |

**2,3-*ortho*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 0.47142 | 2.97406 | -0.77611 |
| C | 1.40124 | 2.05019 | -1.32071 |
| C | 1.53920 | 0.83799 | -0.75294 |
| C | 0.70493 | 0.39540 | 0.35758 |
| C | -0.23407 | 1.37869 | 0.85275 |
| C | -0.33046 | 2.64617 | 0.28160 |
| Br | 1.66216 | -0.41705 | 1.84846 |
| H | 0.08022 | -0.52829 | -0.03564 |
| H | -0.75284 | 1.15202 | 1.77007 |
| H | -1.03883 | 3.35394 | 0.68364 |
| Br | -1.10072 | -2.06760 | -0.62946 |
| Br | -2.92169 | 0.68858 | 0.05160 |
| H | -2.11342 | -0.77698 | -0.33012 |
| H | 2.00588 | 2.31021 | -2.17621 |
| H | 0.40408 | 3.95890 | -1.21709 |
| N | 2.48457 | -0.11560 | -1.36175 |
| O | 2.30530 | -1.28592 | -1.12618 |
| O | 3.35946 | 0.34927 | -2.05965 |

**2,3-*meta*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -1.16229 | 1.29259 | -1.86532 |
| C | -2.88714 | 0.26737 | -0.51710 |
| C | -2.44802 | 0.97190 | -1.70446 |
| C | -1.99179 | -0.28462 | 0.30209 |
| C | -0.15022 | 0.93341 | -0.83661 |
| C | -0.54013 | -0.25823 | 0.02002 |
| H | -3.93891 | 0.18170 | -0.28758 |
| H | 0.83705 | 0.78714 | -1.25846 |
| H | 0.05707 | -0.32015 | 0.92070 |
| Br | 3.35921 | -0.37895 | 0.39067 |
| H | 2.45447 | -1.35967 | -0.10977 |
| Br | 0.08340 | 2.50481 | 0.34815 |
| Br | -0.06127 | -1.91596 | -0.97805 |
| H | -3.18766 | 1.27053 | -2.43243 |
| H | -0.82822 | 1.86860 | -2.71625 |
| N | -2.43719 | -0.99750 | 1.50063 |
| O | -1.57148 | -1.46490 | 2.21233 |
| O | -3.62886 | -1.07591 | 1.70775 |

**2,3-meta-elimination TS3**

| | | | |
|---|---|---|---|
| C | 2.10274 | 0.91469 | 1.65603 |
| C | 0.94865 | 1.35817 | 2.33857 |
| C | -0.21969 | 1.48200 | 1.66706 |
| C | -0.34128 | 1.05921 | 0.27957 |
| C | 0.85129 | 0.54855 | -0.37055 |
| C | 2.04158 | 0.54791 | 0.33755 |
| Br | -1.24579 | 2.37696 | -0.83671 |
| H | -1.11321 | 1.85074 | 2.15085 |
| H | -1.15326 | 0.22521 | 0.29792 |
| H | 0.84881 | 0.35953 | -1.43173 |
| Br | -2.60973 | -1.23569 | 0.35861 |
| Br | 0.52217 | -2.26770 | -0.37171 |
| H | -1.08077 | -1.88945 | -0.00211 |
| H | 1.02029 | 1.62487 | 3.38209 |
| H | 3.05802 | 0.86654 | 2.15961 |
| N | 3.27819 | 0.14134 | -0.35360 |
| O | 3.20517 | -0.02991 | -1.54718 |
| O | 4.27491 | 0.02179 | 0.32375 |

**3,4-*para*-addition TS1**

| | | | |
|---|---|---|---|
| C | 1.73426 | -2.14787 | -0.49766 |
| C | 2.90952 | -0.17220 | 0.07497 |
| C | 2.69747 | -1.54813 | 0.24887 |
| C | 2.20250 | 0.62502 | -0.79596 |
| C | 0.88692 | -1.36627 | -1.38162 |
| C | 1.19071 | 0.04796 | -1.53662 |
| H | 1.54634 | -3.20833 | -0.41709 |
| H | 3.30502 | -2.09470 | 0.95183 |
| H | 0.56370 | -1.85982 | -2.29251 |
| H | 0.67361 | 0.61569 | -2.29288 |
| Br | -0.82798 | 2.02809 | -0.44592 |
| H | -2.26920 | 0.94598 | 0.31449 |
| Br | -0.88492 | -1.41574 | -0.31073 |
| Br | -3.26761 | -0.12544 | 0.85118 |
| H | 2.43079 | 1.67460 | -0.88626 |
| N | 3.99567 | 0.45967 | 0.86783 |
| O | 4.31831 | 1.58331 | 0.56316 |
| O | 4.47787 | -0.20384 | 1.75772 |

**3,4-*para*-addition I1**

| | | | |
|---|---|---|---|
| C | 2.57007 | 0.67950 | -0.13480 |
| C | 0.73057 | 2.21587 | -0.17358 |
| C | 2.12520 | 1.91208 | 0.09724 |
| C | -0.19464 | 1.27956 | -0.37076 |
| C | 1.64956 | -0.32490 | -0.75701 |
| C | 0.20221 | -0.15624 | -0.32367 |
| H | 3.59740 | 0.40415 | 0.04947 |
| H | 2.76343 | 2.69260 | 0.47907 |
| H | 1.64546 | -0.15708 | -1.83838 |
| H | -0.45122 | -0.77509 | -0.92870 |
| Br | -0.15213 | -0.76767 | 1.52915 |
| H | -2.71687 | -0.94888 | 0.60319 |
| Br | 2.29809 | -2.14629 | -0.57904 |
| Br | -3.60231 | -0.75764 | -0.49789 |
| H | -1.23553 | 1.53636 | -0.50073 |
| N | 0.31598 | 3.63157 | -0.16401 |
| O | 1.17586 | 4.45101 | 0.08131 |
| O | -0.84336 | 3.88618 | -0.40232 |

**3,4-met*a*-addition TS1**

| | | | |
|---|---|---|---|
| C | -2.31896 | -0.55777 | 0.94610 |
| C | -2.62702 | 1.38228 | -0.45667 |
| C | -2.96736 | 0.07827 | -0.05949 |
| C | -1.61084 | 2.07259 | 0.17406 |
| C | -1.18160 | 0.09274 | 1.57035 |
| C | -0.88931 | 1.46896 | 1.18271 |
| H | -3.19255 | 1.83724 | -1.25714 |
| H | -1.36614 | 3.07841 | -0.12940 |
| H | -1.03167 | -0.12520 | 2.62206 |
| H | -0.15664 | 2.02135 | 1.74792 |
| Br | 1.76660 | 1.95316 | -0.20726 |
| H | 2.55565 | 0.17711 | -0.48572 |
| Br | 0.30444 | -1.05067 | 0.71742 |
| Br | 2.95848 | -1.32194 | -0.59317 |
| H | -2.61179 | -1.54875 | 1.25858 |
| N | -4.08432 | -0.60573 | -0.73778 |
| O | -4.66190 | 0.01153 | -1.60400 |
| O | -4.34671 | -1.72926 | -0.37461 |

**3,4-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | -2.29041 | 0.11512 | -0.38074 |
| C | -1.11314 | -2.00223 | -0.69247 |
| C | -2.28887 | -1.21414 | -0.36470 |
| C | 0.07798 | -1.40596 | -0.73632 |
| C | -1.04321 | 0.79578 | -0.84183 |
| C | 0.22157 | 0.05135 | -0.44500 |
| H | -1.22890 | -3.06242 | -0.85076 |
| H | 0.98319 | -1.96822 | -0.91691 |
| H | -1.05245 | 0.78416 | -1.93668 |
| H | 1.08259 | 0.48583 | -0.94054 |
| Br | 0.65737 | 0.23317 | 1.48462 |
| H | 3.12414 | -0.43929 | 0.62875 |
| Br | -1.01884 | 2.68324 | -0.39410 |
| Br | 4.00243 | -0.79509 | -0.43787 |
| H | -3.17718 | 0.68050 | -0.13997 |
| N | -3.52651 | -1.92814 | -0.00297 |
| O | -3.48620 | -3.13994 | -0.03367 |
| O | -4.49663 | -1.26874 | 0.29622 |

**3,4-*para*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | 2.70831 | -0.21500 | -1.16686 |
| C | 1.69558 | 1.57507 | 0.02697 |
| C | 2.83580 | 0.99258 | -0.59247 |
| C | 0.45489 | 1.00479 | 0.09114 |
| C | 1.42004 | -0.92661 | -1.13653 |
| C | 0.29132 | -0.24064 | -0.49614 |
| H | -0.37574 | 1.49247 | 0.57714 |
| H | 1.12739 | -1.31109 | -2.11469 |
| H | -0.66249 | -0.73893 | -0.47557 |
| Br | -2.05312 | -0.68861 | 1.63168 |
| H | -2.51356 | 0.09214 | 0.03087 |
| Br | 1.65948 | -2.56300 | -0.04960 |
| Br | -2.62952 | 0.73455 | -1.44117 |
| H | 3.54584 | -0.70365 | -1.64330 |
| H | 3.77125 | 1.52865 | -0.57501 |
| N | 1.88224 | 2.90671 | 0.66051 |
| O | 3.02383 | 3.22686 | 0.90854 |
| O | 0.88946 | 3.55432 | 0.87753 |

**3,4-*para*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -2.49027 | -0.35458 | 0.98882 |
| C | -1.43148 | 1.50975 | -0.09659 |
| C | -2.53630 | 0.93086 | 0.64244 |
| C | -0.26401 | 0.89546 | -0.26785 |
| C | -1.33916 | -1.21294 | 0.60491 |
| C | -0.05786 | -0.44244 | 0.33850 |
| H | 0.54861 | 1.36833 | -0.79837 |
| H | -1.16298 | -2.00977 | 1.31747 |
| H | 0.64982 | -1.03771 | -0.22670 |
| Br | 3.53291 | 0.01929 | -0.95466 |
| H | 3.15034 | 0.04602 | 0.41667 |
| Br | -1.82164 | -2.18501 | -1.05896 |
| Br | 0.87317 | -0.15020 | 2.07598 |
| H | -3.31202 | -0.82027 | 1.51269 |
| H | -3.38169 | 1.55690 | 0.87861 |
| N | -1.61088 | 2.86158 | -0.66011 |
| O | -2.67093 | 3.40919 | -0.44206 |
| O | -0.69868 | 3.33657 | -1.29841 |

**3,4-met*a*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -2.48721 | 0.03101 | -0.77643 |
| C | -1.50716 | -1.51165 | 0.81352 |
| C | -2.62207 | -0.93666 | 0.13970 |
| C | -0.22333 | -1.10741 | 0.54399 |
| C | -1.13715 | 0.52549 | -1.08949 |
| C | -0.01070 | -0.11379 | -0.39524 |
| H | -1.70423 | -2.28043 | 1.54761 |
| H | 0.62568 | -1.54412 | 1.04604 |
| H | -0.95425 | 0.55701 | -2.16510 |
| H | 0.98418 | 0.21379 | -0.64531 |
| Br | 2.50373 | 0.78308 | 1.39925 |
| H | 2.80442 | -0.41817 | 0.19290 |
| Br | -1.07401 | 2.41899 | -0.54118 |
| Br | 2.82721 | -1.55829 | -1.05870 |
| H | -3.34562 | 0.46057 | -1.27153 |
| N | -3.97757 | -1.43011 | 0.47431 |
| O | -4.04814 | -2.29935 | 1.31191 |
| O | -4.90613 | -0.92965 | -0.11432 |

**3,4-met*a*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | 2.23742 | 0.05023 | 0.59132 |
| C | 1.20257 | -1.00623 | -1.35904 |
| C | 2.30338 | -0.78460 | -0.44211 |
| C | -0.00860 | -0.54437 | -1.05136 |
| C | 0.98546 | 0.81097 | 0.82811 |
| C | -0.25230 | 0.16531 | 0.23022 |
| H | 1.39272 | -1.55270 | -2.26884 |
| H | -0.85537 | -0.70823 | -1.70203 |
| H | 0.83859 | 1.03411 | 1.87788 |
| H | -1.06427 | 0.87990 | 0.16023 |
| Br | -3.96541 | -0.07390 | -0.82749 |
| H | -3.28097 | -0.75111 | 0.22373 |
| Br | 1.22752 | 2.59561 | 0.00065 |
| Br | -0.93851 | -1.16573 | 1.55318 |
| H | 3.09366 | 0.21882 | 1.22584 |
| N | 3.57057 | -1.49491 | -0.69939 |
| O | 3.61207 | -2.20015 | -1.68493 |
| O | 4.48145 | -1.33277 | 0.08173 |

**3,4-*para*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 2.49432 | 0.29395 | 0.27641 |
| C | 1.88134 | 1.00935 | 1.33079 |
| C | 0.60817 | 1.42547 | 1.16715 |
| C | -0.15413 | 1.05975 | -0.01934 |
| C | 0.52544 | 0.28906 | -1.03817 |
| C | 1.86528 | -0.06501 | -0.87827 |
| Br | -1.18253 | 2.53154 | -0.77122 |
| H | 0.09879 | 1.98775 | 1.93632 |
| H | -1.02637 | 0.40236 | 0.39667 |
| H | 0.03568 | 0.14002 | -1.98659 |
| H | 2.39218 | -0.60881 | -1.64569 |
| Br | -2.57867 | -0.75169 | 1.11670 |
| Br | -0.36473 | -2.39479 | -0.83561 |
| H | -1.55532 | -1.67676 | 0.18450 |
| H | 2.44706 | 1.22575 | 2.22267 |
| N | 3.92367 | -0.08030 | 0.43631 |
| O | 4.48143 | -0.55532 | -0.52470 |
| O | 4.42201 | 0.12271 | 1.51982 |

**2,5-*ortho*-addition TS1**

| | | | |
|---|---|---|---|
| C | -1.17986 | 1.61532 | 1.94163 |
| C | -1.93561 | 1.42079 | -0.38046 |
| C | -1.29683 | 2.15064 | 0.65580 |
| C | -2.29962 | 0.14571 | -0.13921 |
| C | -1.52898 | 0.31383 | 2.16489 |
| C | -1.98342 | -0.53198 | 1.09132 |
| Br | -0.01724 | -1.30923 | 0.65627 |
| H | -0.76841 | 2.21789 | 2.73639 |
| H | -1.40978 | -0.13339 | 3.14152 |
| H | -2.54707 | -1.42322 | 1.32631 |
| Br | 2.64427 | -1.18644 | -0.33729 |
| H | 2.09353 | 0.33035 | -0.40808 |
| Br | 1.36564 | 1.99471 | -0.44070 |
| H | -1.05234 | 3.18615 | 0.48144 |
| H | -2.11005 | 1.86903 | -1.34553 |
| N | -2.97712 | -0.63112 | -1.19427 |
| O | -3.26641 | -1.77653 | -0.92371 |
| O | -3.20408 | -0.07108 | -2.24080 |

**3,4-met*a*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 2.09952 | -1.49672 | -0.92813 |
| C | 2.36555 | -0.58799 | 0.12568 |
| C | 1.59301 | 0.48809 | 0.35741 |
| C | 0.38728 | 0.68037 | -0.43459 |
| C | 0.12381 | -0.27623 | -1.49370 |
| C | 0.99947 | -1.33665 | -1.72317 |
| Br | 0.15851 | 2.51950 | -1.02578 |
| H | 1.82361 | 1.18311 | 1.15125 |
| H | -0.47739 | 0.60501 | 0.34650 |
| H | -0.66478 | -0.05358 | -2.19356 |
| H | 0.79610 | -2.03013 | -2.52433 |
| Br | -2.02939 | 0.50307 | 1.70856 |
| Br | -2.03491 | -1.92075 | -0.64629 |
| H | -2.13997 | -0.74949 | 0.60885 |
| H | 2.79435 | -2.30793 | -1.08933 |
| N | 3.56434 | -0.81185 | 0.96055 |
| O | 3.76126 | -0.03898 | 1.86792 |
| O | 4.26479 | -1.75517 | 0.66694 |

**2,5-*meta*-addition TS1**

| | | | |
|---|---|---|---|
| C | 1.52256 | 0.58179 | 2.12270 |
| C | 2.26418 | 0.30730 | -0.17067 |
| C | 2.06080 | -0.23676 | 1.10817 |
| C | 1.79924 | 1.53303 | -0.51285 |
| C | 1.05856 | 1.81970 | 1.81871 |
| C | 1.05108 | 2.29639 | 0.45341 |
| Br | -0.88758 | 1.58195 | -0.15066 |
| H | 1.44925 | 0.19074 | 3.12548 |
| H | 0.61866 | 2.44865 | 2.57965 |
| H | 0.97647 | 3.36277 | 0.29089 |
| Br | -2.91579 | -0.37372 | -0.52896 |
| H | -1.61556 | -1.18413 | 0.02409 |
| Br | -0.12275 | -1.98523 | 0.62886 |
| H | 2.49431 | -1.19640 | 1.33642 |
| H | 1.93886 | 1.90789 | -1.51610 |
| N | 2.98195 | -0.49618 | -1.17469 |
| O | 3.02521 | -0.06074 | -2.30352 |
| O | 3.49232 | -1.52303 | -0.79122 |

**2,5-*ortho*-addition I1**

| | | | |
|---|---|---|---|
| C | 0.48171 | -0.61922 | 1.53614 |
| C | -0.26312 | -2.71643 | -0.20646 |
| C | -0.78285 | -0.72829 | 1.16056 |
| C | 1.00795 | -2.63270 | 0.15821 |
| C | 1.52804 | -1.50827 | 0.97566 |
| C | -1.27907 | -1.68875 | 0.14713 |
| H | 0.76112 | 0.11898 | 2.27368 |
| H | -0.60806 | -3.54063 | -0.81498 |
| H | 1.72024 | -3.38726 | -0.14462 |
| H | -2.22435 | -2.12454 | 0.45133 |
| Br | -1.75039 | -0.71342 | -1.51587 |
| Br | 2.74558 | -0.39609 | -0.14191 |
| Br | 0.16096 | 2.84350 | -0.38248 |
| H | 0.91866 | 1.68912 | -0.72375 |
| H | 2.19629 | -1.85227 | 1.76031 |
| N | -1.79165 | 0.12436 | 1.82176 |
| O | -2.95375 | -0.14577 | 1.60404 |
| O | -1.40166 | 1.00809 | 2.54940 |

**2,5-*ortho*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -0.88909 | -0.34161 | -1.52887 |
| C | 0.45728 | 0.45893 | 0.26981 |
| C | 0.32934 | -0.21553 | -0.95960 |
| C | -0.66967 | 1.04646 | 0.91995 |
| C | -2.10957 | 0.20375 | -0.90743 |
| C | -1.87345 | 0.93563 | 0.34578 |
| H | -1.01921 | -0.87329 | -2.46117 |
| H | -0.54686 | 1.58033 | 1.85014 |
| H | -2.70638 | 0.79715 | -1.59896 |
| Br | 2.84488 | -1.58005 | 0.91889 |
| H | 3.25690 | -0.14823 | 0.06971 |
| Br | -3.26213 | -1.35092 | -0.49980 |
| Br | 3.37306 | 1.34975 | -0.74205 |
| H | 1.21705 | -0.62752 | -1.41279 |
| H | 1.42336 | 0.55150 | 0.73238 |
| N | -3.03359 | 1.62432 | 0.95153 |
| O | -3.93140 | 1.91767 | 0.19392 |
| O | -2.98263 | 1.85318 | 2.13429 |

**2,5-*meta*-addition I1**

| | | | |
|---|---|---|---|
| C | 0.61860 | -0.88443 | 1.15928 |
| C | -1.44451 | -2.43566 | 0.07506 |
| C | -0.61734 | -0.58449 | 1.52812 |
| C | -0.19997 | -2.71131 | -0.28602 |
| C | 0.96249 | -1.87384 | 0.11198 |
| C | -1.78838 | -1.26904 | 0.92780 |
| H | -2.26419 | -3.05772 | -0.25629 |
| H | -0.78218 | 0.16320 | 2.29029 |
| H | 0.01576 | -3.55959 | -0.92046 |
| H | -2.50553 | -1.53536 | 1.69965 |
| Br | -2.78886 | 0.06047 | -0.15028 |
| Br | 1.60673 | -0.92361 | -1.51873 |
| Br | 0.35340 | 2.83859 | -0.34316 |
| H | 0.56139 | 1.55658 | -0.92704 |
| H | 1.82854 | -2.46218 | 0.39388 |
| N | 1.74388 | -0.23400 | 1.85925 |
| O | 2.85057 | -0.67550 | 1.63003 |
| O | 1.49434 | 0.66862 | 2.62422 |

**2,5-*meta*-isomerisation TS2**

| | | | |
|---|---|---|---|
| C | -1.33198 | -1.06342 | -1.23730 |
| C | 0.17615 | 0.40816 | -0.10845 |
| C | -0.08886 | -0.80497 | -0.78332 |
| C | -0.86083 | 1.35195 | 0.08088 |
| C | -2.44074 | -0.10850 | -1.05809 |
| C | -2.11231 | 1.14314 | -0.35779 |
| H | -1.55656 | -1.98816 | -1.75010 |
| H | -2.92729 | 0.11041 | -2.01099 |
| H | -2.88371 | 1.88415 | -0.20104 |
| Br | 2.31337 | -1.29954 | 1.51993 |
| H | 2.84636 | -0.57552 | 0.03132 |
| Br | -3.86516 | -0.98049 | -0.00639 |
| Br | 3.08182 | 0.23155 | -1.43004 |
| H | 0.72283 | -1.50395 | -0.90544 |
| H | 1.15741 | 0.63133 | 0.27418 |
| N | -0.55204 | 2.61626 | 0.79444 |
| O | -1.46492 | 3.40117 | 0.92420 |
| O | 0.57816 | 2.75713 | 1.18365 |

**2,5-*ortho*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | -0.78339 | -0.92247 | -1.34568 |
| C | 0.60948 | 0.43622 | 0.16871 |
| C | 0.41435 | -0.58552 | -0.89056 |
| C | -0.63776 | 1.09180 | 0.63012 |
| C | -2.05208 | -0.34373 | -0.82943 |
| C | -1.82071 | 0.74141 | 0.15212 |
| H | -0.88323 | -1.68348 | -2.10690 |
| H | -2.71988 | -0.02316 | -1.62213 |
| Br | 4.11348 | -1.24658 | 0.46375 |
| H | 3.79699 | 0.08077 | 0.05153 |
| Br | -3.07186 | -1.80608 | 0.04603 |
| Br | 1.80665 | 1.87055 | -0.52134 |
| H | 1.30425 | -1.06029 | -1.27948 |
| H | 1.18006 | 0.04157 | 1.00752 |
| H | -0.56848 | 1.88740 | 1.35744 |
| N | -3.00288 | 1.51575 | 0.57998 |
| O | -3.97560 | 1.45624 | -0.14092 |
| O | -2.91920 | 2.17058 | 1.59407 |

**2,5-*ortho*-elimination TS3**

| | | | |
|---|---|---|---|
| C | -0.82785 | -1.19265 | -0.26759 |
| C | 0.96329 | -1.80679 | 1.17753 |
| C | 0.23008 | -1.99034 | -0.01752 |
| C | 0.52433 | -0.90555 | 2.16136 |
| C | -1.17954 | -0.08506 | 0.60655 |
| C | -0.54494 | -0.11004 | 1.90914 |
| H | 1.04966 | -0.84226 | 3.10160 |
| H | -0.55874 | 0.80083 | 0.10732 |
| H | -0.89616 | 0.60033 | 2.64379 |
| Br | 0.94922 | 2.03768 | -0.59186 |
| H | 2.07871 | 0.80558 | -0.27062 |
| Br | -3.01535 | 0.49353 | 0.64319 |
| Br | 3.19063 | -0.47045 | 0.06542 |
| H | 1.76466 | -2.49175 | 1.40132 |
| H | 0.53004 | -2.73788 | -0.73515 |
| N | -1.50130 | -1.33972 | -1.56787 |
| O | -1.78375 | -0.32063 | -2.14731 |
| O | -1.69231 | -2.47196 | -1.94972 |

**2,5-*meta*-isomerisation I2**

| | | | |
|---|---|---|---|
| C | 1.30703 | -1.31065 | 1.00348 |
| C | -0.34356 | 0.24582 | 0.01462 |
| C | 0.06225 | -1.03955 | 0.63972 |
| C | 0.81034 | 1.12006 | -0.29390 |
| C | 2.43132 | -0.36100 | 0.79546 |
| C | 2.06039 | 0.87586 | 0.06525 |
| H | 1.54613 | -2.25573 | 1.47021 |
| H | 2.93158 | -0.12119 | 1.73187 |
| H | 2.83800 | 1.57877 | -0.19563 |
| Br | -3.76080 | -1.50235 | -0.65841 |
| H | -3.44850 | -0.36586 | 0.14386 |
| Br | 3.86003 | -1.26007 | -0.24095 |
| Br | -1.54849 | 1.19147 | 1.29561 |
| H | -0.72921 | -1.75651 | 0.80915 |
| H | -0.98239 | 0.10521 | -0.85143 |
| N | 0.53542 | 2.32557 | -1.10047 |
| O | -0.51885 | 2.34603 | -1.69860 |
| O | 1.37559 | 3.19599 | -1.12909 |

**2,5-*meta*-elimination TS3**

| | | | |
|---|---|---|---|
| C | 0.67708 | 1.31153 | -0.43975 |
| C | -1.07400 | 1.25557 | 1.22198 |
| C | -0.55110 | 1.67998 | -0.01563 |
| C | -0.22955 | 0.58155 | 2.12981 |
| C | 1.44508 | 0.39754 | 0.37315 |
| C | 1.01263 | 0.20378 | 1.74478 |
| H | 1.04073 | 1.61983 | -1.40914 |
| H | -0.60134 | 0.34804 | 3.11532 |
| H | 1.07274 | -0.63857 | -0.09483 |
| H | 1.66352 | -0.34370 | 2.41110 |
| Br | 0.16329 | -2.37318 | -0.73976 |
| H | -1.25858 | -1.63183 | -0.19676 |
| Br | 3.34439 | 0.39904 | 0.07336 |
| Br | -2.67554 | -0.80884 | 0.37019 |
| H | -2.02726 | 1.64533 | 1.53729 |
| N | -1.38255 | 2.54603 | -0.87225 |
| O | -2.40672 | 2.96832 | -0.38767 |
| O | -0.97051 | 2.78209 | -1.98435 |