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# Transition state geometry prediction using molecular group contributions

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In this PDF document:

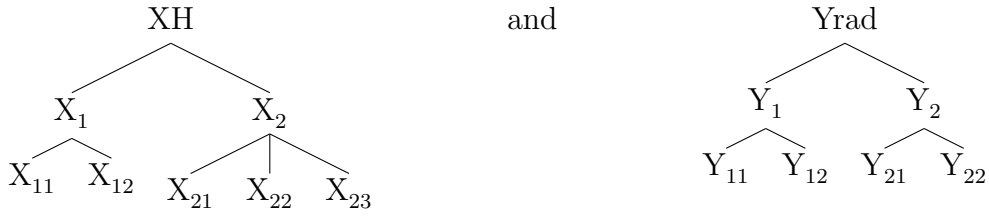


In other supplementary info files:

- 3D geometries of optimized and validated transition states in CML format
- Training data and trained group values and definitions in RMG-Py format

## Group Training Regression Details

Consider the trees:




and a known transition state that matches nodes $X_{11}$ and $Y_{22}$. This example will deal with a single distance $d$, but in reality it is done for each of the three distances dXH, dHY, and dXY. The distance $d_{11,22}$ from the known transition state can be used to train the groups ($X_{11}$,$Y_{22}$) and all combinations of the ancestors of these groups, namely ($X_{11}$,$Y_2$), ($X_{11}$,Yrad), ($X_1$,$Y_{22}$), ($X_1$,$Y_2$), ($X_1$,Yrad), (XH,$Y_{22}$), (XH,$Y_2$), and (XH,Yrad). If a second known transition state matches nodes ($X_{23}$,$Y_2$) and has distance $d_{23,2}$ then it provides data for those groups ($X_{23}$,$Y_2$) and all the pairs of ancestors: ($X_{23}$,Yrad), ($X_2$,$Y_2$), ($X_2$,Yrad), (XH,$Y_2$), and (XH,Yrad).

From the two training transition states with distances $d_{11,22}$ and $d_{23,2}$ we construct a set of 15 linear equations,

$$X_{11} + Y_{22} + d_0 = d_{11,22} \quad (1)$$
$$X_{11} + Y_2 + d_0 = d_{11,22} \quad (2)$$
$$X_{11} + \mathrm{Yrad} + d_0 = d_{11,22} \quad (3)$$
$$X_1 + Y_{22} + d_0 = d_{11,22} \quad (4)$$
$$X_1 + Y_2 + d_0 = d_{11,22} \quad (5)$$
$$X_1 + \mathrm{Yrad} + d_0 = d_{11,22} \quad (6)$$
$$\mathrm{XH} + Y_{22} + d_0 = d_{11,22} \quad (7)$$
$$\mathrm{XH} + Y_2 + d_0 = d_{11,22} \quad (8)$$
$$\mathrm{XH} + \mathrm{Yrad} + d_0 = d_{11,22} \quad (9)$$
$$X_{23} + Y_2 + d_0 = d_{23,2} \quad (10)$$
$$X_{23} + \mathrm{Yrad} + d_0 = d_{23,2} \quad (11)$$
$$X_2 + Y_2 + d_0 = d_{23,2} \quad (12)$$
$$X_2 + \mathrm{Yrad} + d_0 = d_{23,2} \quad (13)$$
$$\mathrm{XH} + Y_2 + d_0 = d_{23,2} \quad (14)$$
$$\mathrm{XH} + \mathrm{Yrad} + d_0 = d_{23,2} \quad (15)$$

where $d_0$ is the base distance common to all transition states, so that the final group values contain only deviations from the base value.

This set of 15 equations in 9 unknowns is over-specified, for example equations (8) and (14) have the same left hand side, and equations (9) and (15) are also duplicates. Indeed, every known transition state will lead to an expression like (9) and (15) for $\mathrm{XH} + \mathrm{Yrad} + d_0$. Although there is not a set of group values ($X_{11}$, $X_1$, Xrad, $Y_{22}$, etc.) that will precisely

solve the above set of linear equations, we can find the values that minimize the error in the equations in the least-squares sense. This is the form of the linear least squares regression used to train the group values.

Writing the above set of equations in matrix form:

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \mathrm{XH} \\ \mathrm{X}_1 \\ \mathrm{X}_2 \\ \mathrm{X}_{11} \\ \mathrm{X}_{23} \\ \mathrm{Yrad} \\ \mathrm{Y}_2 \\ \mathrm{Y}_{22} \\ d_0 \end{bmatrix} = \begin{bmatrix} d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{11,22} \\ d_{23,2} \\ d_{23,2} \\ d_{23,2} \\ d_{23,2} \\ d_{23,2} \\ d_{23,2} \end{bmatrix} \tag{16}$$

we can use the notation

$$\mathbf{X} \cdot \beta = y \tag{17}$$

The least-squares fitted group values in the vector $\beta$ can be found by

$$\beta = \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{X}^T y \tag{18}$$

or using Numpy's linear algebra library in Python:

```
beta, residues, rank, s = numpy.linalg.lstsq(X, y)
```

which computes the vector $\beta$ that minimizes the Euclidean 2-norm

$$\|y - \mathbf{X}\beta\|^2 \tag{19}$$

## Predicted vs Optimized distances

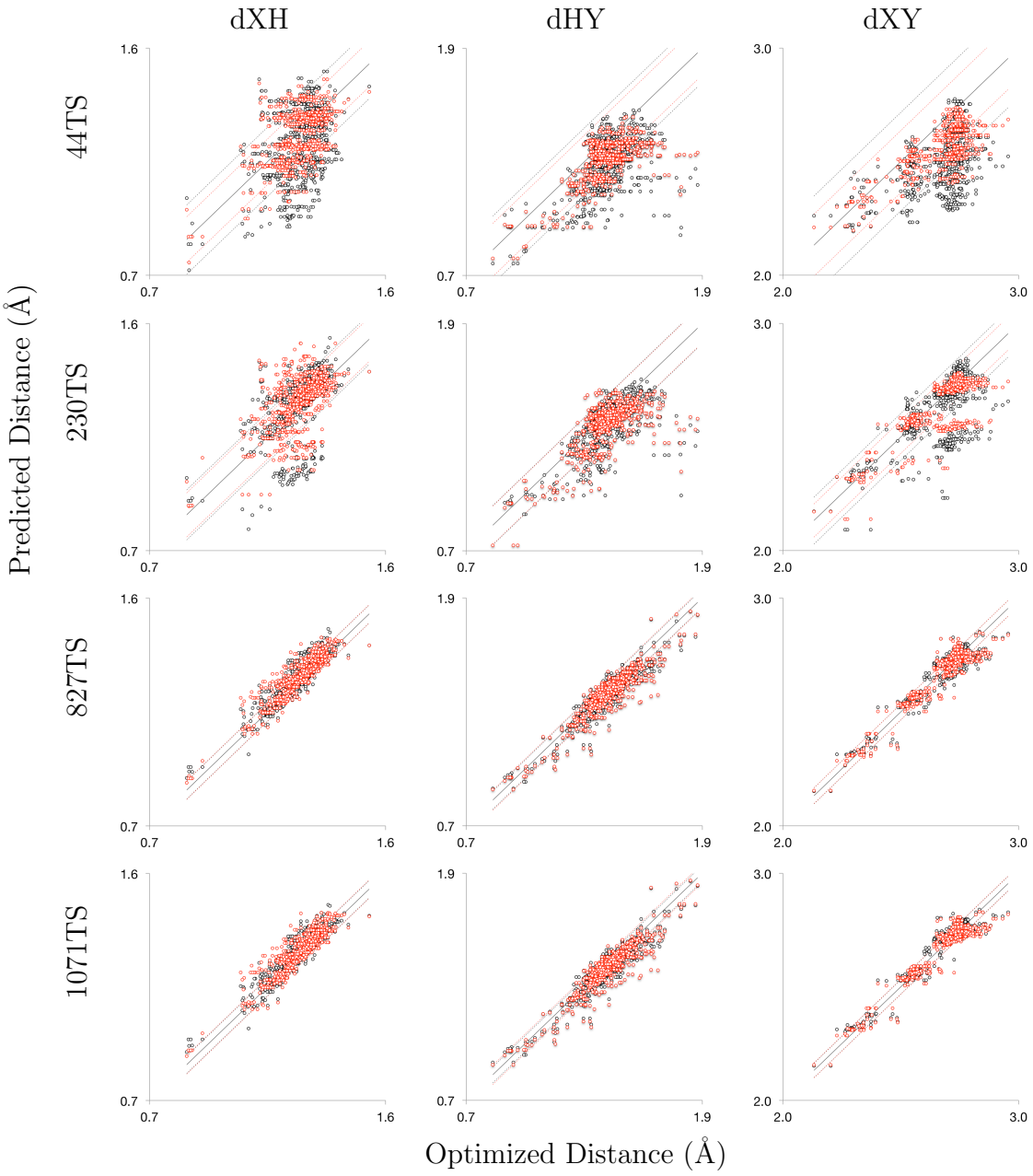



Figure 1: Comparison of distances from validated transition states to predictions from molecular group values calculated from different sized data sets. The solid line represents parity, the dashed lines represent the root mean squared error of the estimates from parity. The predictions derived from the original and new trees are represented by the black and red circles respectively.

## Group Naming Convention

While much detail is included in molecular group names, a full description of the group should be checked in the *TS_groups.py* file. Atoms where the element is undefined are typically assigned as an *R* atom, unless the atom is reactive where it is assigned as either *X* or *Y*.

Molecular group names assume radical count is zero if undefined. For example, if radicals are not included in the name, the atom has no radical electrons. So the group *X_H* describes a molecular group where a hydrogen atom is bonded to an atom X which does not have any unpaired (radical) electrons.

Atom bonding is described by the letters *s*, *d*, *dd*, *t*, and *b*: *s* mean the atom only has single bonds, *d* means the atom has exactly one double bond, *dd* means the atom has 2 double bonds, *t* means the atom has a triple bond, and *b* means the atom is part of an aromatic ring. Thus *Cs* signifies Carbon atom with only single bonds (not a caesium atom).

A forward slash denotes atoms bonded to the atom specified before the first forward slash. For example, *C/H3/Cs* describes a carbon atom, bonded to 3 hydrogen atoms and to a carbon with only single bonds.

A backslash has the same meaning as the forward slash, but the atom being considered is before the first backslash. For example, *C/H3/Cs\H2\Cs* describes a carbon atom bonded to 3 hydrogen atoms and to a carbon which has single bonds to 2 hydrogen atoms and a third carbon (which only has single bonds).

## Group values for original tree

Table 1: Original tree structure, with distance group data in Å.

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L1: X_H_or_Xanyrad_H | 2142 | 1.336010 | 1.336330 | 2.667560 |
| L2: X_H | 2089 | -0.002556 | 0.002864 | 0.000227 |
| L3: H2 | 70 | -0.327434 | -0.045046 | -0.369886 |
| L3: Ct_H | 12 | 0.426157 | -0.214467 | 0.120589 |
| L4: Ct/H/NonDeC | 12 | 0.426157 | -0.214467 | 0.120589 |
| L3: O_H | 203 | -0.110714 | -0.034542 | -0.149127 |
| L4: O_pri | 14 | 0.075716 | -0.199700 | -0.158817 |
| L4: O_sec | 189 | -0.122296 | -0.024281 | -0.148525 |
| L5: O/H/NonDeC | 51 | -0.061770 | -0.091698 | -0.156862 |
| L5: O/H/NonDeO | 137 | -0.143000 | -0.000215 | -0.144650 |
| L6: H2O2 | 37 | -0.172464 | 0.030481 | -0.143076 |
| L6: ROOH_pri | 31 | -0.164228 | 0.023011 | -0.141922 |
| L6: ROOH_sec | 1 | -0.023183 | -0.146971 | -0.174787 |
| L6: ROOH_ter | 1 | -0.216642 | 0.096657 | -0.117164 |
| L5: O/H/OneDe | 1 | -0.241135 | -0.138830 | -0.383406 |
| L6: O/H/OneDeC | 1 | -0.241135 | -0.138830 | -0.383406 |
| L3: Orad_O_H | 22 | -0.244636 | 0.181811 | -0.064615 |
| L3: Cd_H | 319 | 0.085747 | -0.068103 | 0.017934 |
| L4: Cd_pri | 210 | 0.080833 | -0.065760 | 0.015103 |
| L5: Cd/H2/NonDeC | 210 | 0.080833 | -0.065760 | 0.015103 |
| L4: Cd_sec | 109 | 0.095340 | -0.072680 | 0.023461 |
| L5: Cd/H/NonDeC | 30 | 0.072086 | -0.053192 | 0.015788 |
| L5: Cd/H/NonDeO | | | | |
| L5: Cd/H/OneDe | 79 | 0.104163 | -0.080074 | 0.026373 |
| L6: Cd/H/Ct | 26 | 0.033884 | -0.029006 | 0.006386 |
| L6: Cd/H/Cb | | | | |
| L6: Cd/H/CO | | | | |
| L6: Cd/H/Cd | 53 | 0.139835 | -0.105994 | 0.036518 |
| L3: Cb_H | 44 | 0.124436 | -0.092331 | 0.033127 |
| L3: CO_H | 153 | -0.001372 | 0.059389 | 0.057711 |
| L4: CO_pri | 50 | 0.000467 | 0.049726 | 0.050841 |
| L4: CO_sec | 103 | -0.002287 | 0.064195 | 0.061127 |
| L5: CO/H/NonDe | 60 | -0.009196 | 0.071787 | 0.062334 |
| L6: CO/H/Cs | 55 | -0.009637 | 0.077298 | 0.067136 |
| L7: CO/H/Cs\Cs—Cs | 6 | -0.039990 | 0.127041 | 0.088998 |
| L5: CO/H/OneDe | 43 | 0.006808 | 0.054200 | 0.059539 |
| L3: Cs_H | 1266 | 0.007461 | 0.023642 | 0.032296 |
| L4: C_methane | 69 | 0.076680 | -0.051468 | 0.028801 |
| L4: C_pri | 684 | 0.025511 | -0.002230 | 0.025031 |
| L5: C/H3/Cs | 357 | 0.051887 | -0.033063 | 0.021528 |
| L6: C/H3/Cs\H3 | 65 | 0.045880 | -0.025075 | 0.024181 |
| L6: C/H3/Cs\OneNonDe | 107 | 0.053158 | -0.037890 | 0.017928 |
| L7: C/H3/Cs\H2\Cs | 59 | 0.049403 | -0.042001 | 0.010665 |
| L8: C/H3/Cs\H2\Cs—O | 1 | 0.045526 | -0.296175 | -0.246802 |
| L7: C/H3/Cs\H2\O | 48 | 0.057673 | -0.032947 | 0.026660 |

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**Table 1 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L6: C/H3/Cs\TwoNonDe | 44 | 0.049381 | -0.031488 | 0.021282 |
| L7: C/H3/Cs\H\Cs\O | | | | |
| L7: C/H3/Cs\H\Cs\Cs—O | | | | |
| L5: C/H3/O | 53 | 0.025187 | 0.000259 | 0.020403 |
| L5: C/H3/OneDe | 274 | -0.007707 | 0.036215 | 0.030303 |
| L6: C/H3/Ct | 36 | -0.003456 | 0.024269 | 0.023000 |
| L6: C/H3/Cb | | | | |
| L6: C/H3/CO | 84 | 0.012344 | 0.003831 | 0.016124 |
| L6: C/H3/Cd | 154 | -0.019271 | 0.056043 | 0.039454 |
| L7: C/H3/Cd\H_Cd\H2 | 46 | -0.022590 | 0.051658 | 0.031290 |
| L7: C/H3/Cd\H_Cd\H\Cs | 3 | -0.047979 | 0.075930 | 0.031408 |
| L7: C/H3/Cd\Cs_Cd\H2 | 3 | -0.023917 | 0.029891 | 0.010253 |
| L4: C_sec | 409 | -0.026003 | 0.069757 | 0.044341 |
| L5: C/H2/NonDeC | 73 | 0.027438 | -0.019733 | 0.010886 |
| L6: C/H2/Cs/Cs\O | | | | |
| L6: C/H2/Cs/Cs\Cs—O | | | | |
| L6: C/H2/NonDeC_5ring | 5 | -0.018316 | -0.013568 | -0.027701 |
| L7: C/H2/NonDeC_5ring_fused6_1 | | | | |
| L7: C/H2/NonDeC_5ring_fused6_2 | | | | |
| L7: C/H2/NonDeC_5ring_alpha6ring | | | | |
| L7: C/H2/NonDeC_5ring_beta6ring | | | | |
| L6: C/H2/Cs\H3/Cs\H3 | 53 | 0.037209 | -0.011011 | 0.029214 |
| L5: C/H2/NonDeO | 52 | 0.011534 | 0.020231 | 0.027527 |
| L6: C/H2/CsO | 50 | 0.010769 | 0.021611 | 0.027966 |
| L7: C/H2/Cs\Cs2/O | | | | |
| L6: C/H2/O2 | 2 | 0.031818 | -0.016339 | 0.015885 |
| L5: C/H2/OneDe | 185 | -0.037737 | 0.086334 | 0.048927 |
| L6: C/H2/OneDeC | 184 | -0.037603 | 0.086091 | 0.048826 |
| L7: C/H2/CtCs | | | | |
| L7: C/H2/CbCs | | | | |
| L7: C/H2/COCs | 41 | -0.014812 | 0.053991 | 0.038405 |
| L8: C/H2/CO\H/Cs\H3 | 1 | -0.050355 | 0.095460 | 0.047057 |
| L7: C/H2/CdCs | 143 | -0.043987 | 0.095083 | 0.051745 |
| L8: C/H2/Cd\H_Cd\H2/Cs\H3 | 33 | -0.029127 | 0.076789 | 0.049531 |
| L6: C/H2/OneDeO | 1 | -0.059511 | 0.125879 | 0.065513 |
| L5: C/H2/TwoDe | 99 | -0.060370 | 0.126094 | 0.067502 |
| L6: C/H2/CtCt | | | | |
| L6: C/H2/CtCb | | | | |
| L6: C/H2/CtCO | | | | |
| L6: C/H2/CbCb | | | | |
| L6: C/H2/CbCO | | | | |
| L6: C/H2/COCO | | | | |
| L6: C/H2/CdCt | | | | |
| L6: C/H2/CdCb | | | | |
| L6: C/H2/CdCO | | | | |
| L6: C/H2/CdCd | 99 | -0.060370 | 0.126094 | 0.067502 |
| L5: C/H2/Cb | | | | |
| L4: C_ter | 104 | -0.025676 | 0.062321 | 0.034956 |

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**Table 1 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L5: C/H/NonDe | 16 | 0.001573 | 0.003478 | 0.006838 |
| L6: C/H/Cs3 | 15 | 0.006985 | 0.005657 | 0.014344 |
| L7: C/H/Cs3_5ring | | | | |
| L8: C/H/Cs3_5ring_fused6 | | | | |
| L8: C/H/Cs3_5ring_adj5 | | | | |
| L7: C/H/Cs2/Cs\O | | | | |
| L6: C/H/NDMustO | 1 | -0.128313 | -0.048800 | -0.173313 |
| L7: C/H/Cs2O | 1 | -0.128313 | -0.048800 | -0.173313 |
| L7: C/H/CsO2 | | | | |
| L7: C/H/O3 | | | | |
| L5: C/H/OneDe | 87 | -0.029273 | 0.070037 | 0.038474 |
| L6: C/H/Cs2 | 87 | -0.029273 | 0.070037 | 0.038474 |
| L7: C/H/Cs2Ct | | | | |
| L7: C/H/Cs2Cb | | | | |
| L7: C/H/Cs2CO | 87 | -0.029273 | 0.070037 | 0.038474 |
| L7: C/H/Cs2Cd | | | | |
| L6: C/H/CsO | | | | |
| L6: C/H/OO | | | | |
| L5: C/H/TwoDe | 1 | -0.119337 | 0.270561 | 0.154144 |
| L6: C/H/Cs | 1 | -0.119337 | 0.270561 | 0.154144 |
| L7: C/H/CtCt | | | | |
| L7: C/H/CtCb | | | | |
| L7: C/H/CtCO | | | | |
| L7: C/H/CbCb | | | | |
| L7: C/H/CbCO | | | | |
| L7: C/H/COCO | | | | |
| L7: C/H/CdCt | | | | |
| L7: C/H/CdCb | | | | |
| L7: C/H/CdCO | | | | |
| L7: C/H/CdCd | 1 | -0.119337 | 0.270561 | 0.154144 |
| L6: C/H/TDMustO | | | | |
| L5: C/H/ThreeDe | | | | |
| L5: C/H/Cb | | | | |
| L2: Xrad_H | 53 | 0.094987 | -0.106435 | -0.008430 |
| L3: C_rad_H | 38 | 0.155959 | -0.117206 | 0.041719 |
| L4: CH3_rad_H | 38 | 0.155959 | -0.117206 | 0.041719 |
| L3: OH_rad_H | 15 | -0.074639 | -0.076468 | -0.147944 |
| L2: Xbirad_H | | | | |
| L3: CH2_triplet_H | | | | |
| L3: CH2_singlet_H | | | | |
| L2: Xtrirad_H | | | | |
| L3: C_quartet_H | | | | |
| L3: C_doublet_H | | | | |
| L1: Y_anyrad | | | | |
| L2: Y_1centerquadrad | | | | |
| L3: C_quintet | | | | |
| L3: C_triplet | | | | |
| L3: C_singlet | | | | |

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**Table 1 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L2: Y_1centertrirad | | | | |
| L3: CH_quartet | | | | |
| L3: CH_doublet | | | | |
| L2: Y_1centerbirad | 53 | -0.106387 | 0.093103 | -0.010316 |
| L3: O_atom_triplet | 15 | -0.078856 | -0.073302 | -0.149113 |
| L3: O_atom_singlet | | | | |
| L3: CH2_triplet | 38 | -0.116742 | 0.155689 | 0.041886 |
| L3: CH2_singlet | | | | |
| L2: Y_rad | 2089 | 0.002857 | -0.002500 | 0.000277 |
| L3: H_rad | 70 | -0.044160 | -0.330263 | -0.371926 |
| L3: Y_2centeradjbirad | 22 | 0.183054 | -0.244770 | -0.063414 |
| L4: O2b | 22 | 0.183054 | -0.244770 | -0.063414 |
| L4: C2b | | | | |
| L3: Ct_rad | 12 | -0.215601 | 0.427396 | 0.121746 |
| L4: Ct_rad/Ct | 12 | -0.215601 | 0.427396 | 0.121746 |
| L3: O_rad | 203 | -0.035877 | -0.108766 | -0.148471 |
| L4: O_pri_rad | 14 | -0.200121 | 0.080838 | -0.153831 |
| L4: O_sec_rad | 189 | -0.024990 | -0.121335 | -0.148115 |
| L5: O_rad/NonDeC | 51 | -0.091751 | -0.061514 | -0.156592 |
| L6: O_rad/Cs\H2\Cs—H—Cs2 | | | | |
| L5: O_rad/NonDeO | 137 | 0.000232 | -0.143066 | -0.144048 |
| L6: OOC | 100 | -0.009950 | -0.133086 | -0.144316 |
| L5: O_rad/OneDe | 1 | -0.139436 | -0.241161 | -0.384069 |
| L6: O_rad/OneDeC | 1 | -0.139436 | -0.241161 | -0.384069 |
| L7: O_rad/Cd | | | | |
| L8: O_rad/Cd\H_Cd\H2 | | | | |
| L8: O_rad/Cd\H_Cd\H\Cs | | | | |
| L8: O_rad/Cd\H_Cd\Cs2 | | | | |
| L8: O_rad/Cd\Cs_Cd\H2 | | | | |
| L8: O_rad/Cd\Cs_Cd\H\Cs | | | | |
| L8: O_rad/Cd\Cs_Cd\Cs2 | | | | |
| L3: Cd_rad | 319 | -0.068341 | 0.085680 | 0.017720 |
| L4: Cd_pri_rad | 210 | -0.065901 | 0.080755 | 0.014975 |
| L5: Cd_Cd\H2_pri_rad | 37 | -0.090673 | 0.111803 | 0.024431 |
| L5: Cd_Cd\H\Cs_pri_rad | 25 | -0.084518 | 0.116254 | 0.030054 |
| L6: Cd_Cd\H\Cs—H2—Cs_pri_rad | | | | |
| L5: Cd_Cd\Cs2_pri_rad | | | | |
| L4: Cd_sec_rad | 109 | -0.073073 | 0.095230 | 0.023044 |
| L5: Cd_rad/NonDeC | 30 | -0.053245 | 0.071823 | 0.015883 |
| L6: Cd_Cd\H2_rad/Cs | 29 | -0.047865 | 0.071398 | 0.020717 |
| L6: Cd_Cd\H\Cs_rad/Cs | 1 | -0.338387 | 0.094328 | -0.240337 |
| L5: Cd_rad/NonDeO | | | | |
| L5: Cd_rad/OneDe | 79 | -0.080561 | 0.104069 | 0.025748 |
| L6: Cd_rad/Ct | 26 | -0.028430 | 0.033281 | 0.006395 |
| L6: Cd_rad/Cb | | | | |
| L6: Cd_rad/CO | | | | |
| L6: Cd_rad/Cd | 53 | -0.106627 | 0.139463 | 0.035425 |
| L3: Cb_rad | 44 | -0.092544 | 0.124820 | 0.033389 |

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**Table 1 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L3: CO_rad | 153 | 0.060690 | -0.001930 | 0.058483 |
| L4: CO_pri_rad | 50 | 0.051903 | -0.000963 | 0.051657 |
| L4: CO_sec_rad | 103 | 0.064999 | -0.002404 | 0.061831 |
| L5: CO_rad/NonDe | 60 | 0.072193 | -0.008661 | 0.063342 |
| L5: CO_rad/OneDe | 43 | 0.055533 | 0.005830 | 0.059842 |
| L3: Cs_rad | 1266 | 0.024200 | 0.007289 | 0.032625 |
| L4: C_methyl | 69 | -0.050813 | 0.075919 | 0.028607 |
| L4: C_pri_rad | 684 | -0.001792 | 0.025273 | 0.025176 |
| L5: C_rad/H2/Cs | 357 | -0.032772 | 0.051719 | 0.021617 |
| L6: C_rad/H2/Cs\H3 | 65 | -0.024753 | 0.045959 | 0.024509 |
| L6: C_rad/H2/Cs\Cs2\O | 2 | -0.125966 | 0.025305 | -0.097425 |
| L6: C_rad/H2/Cs\H\Cs\Cs—O | 31 | -0.033915 | 0.057010 | 0.024538 |
| L6: C_rad/H2/Cs\H\Cs—Cs\O | | | | |
| L6: C_rad/H2/Cs\H2\Cs—Cs—O | | | | |
| L6: C_rad/H2/Cs\H2\Cs—Cs#O | 1 | -0.296450 | 0.035505 | -0.257321 |
| L5: C_rad/H2/Ct | 36 | 0.026030 | -0.004893 | 0.023289 |
| L5: C_rad/H2/Cb | | | | |
| L5: C_rad/H2/CO | 84 | 0.004886 | 0.011458 | 0.016257 |
| L5: C_rad/H2/O | 53 | 0.000911 | 0.024796 | 0.020406 |
| L5: C_rad/H2/Cd | 154 | 0.056969 | -0.019724 | 0.039836 |
| L6: C_rad/H2/Cd\H_Cd\H2 | 118 | 0.058876 | -0.021124 | 0.040298 |
| L6: C_rad/H2/Cd\Cs_Cd\H2 | 3 | 0.030025 | -0.024190 | 0.010083 |
| L4: C_sec_rad | 409 | 0.070550 | -0.026112 | 0.044984 |
| L5: C_rad/H/NonDeC | 73 | -0.018369 | 0.026681 | 0.011442 |
| L6: C_rad/H/NonDeC_5ring_fused6_1 | | | | |
| L6: C_rad/H/NonDeC_5ring_fused6_2 | | | | |
| L6: C_rad/H/Cs\H3/Cs\H3 | 53 | -0.010088 | 0.036102 | 0.028957 |
| L6: C_rad/H/NonDeC_5ring_alpha6ring | | | | |
| L6: C_rad/H/NonDeC_5ring_beta6ring | | | | |
| L6: C_rad/H/Cs\H2\Cs/Cs\H2\O | | | | |
| L6: C_rad/H/Cs\H\Cs\O/Cs | | | | |
| L6: C_rad/H/Cs\H2\Cs—O/Cs | | | | |
| L5: C_rad/H/NonDeO | 52 | 0.020310 | 0.011913 | 0.027769 |
| L6: C_rad/H/CsO | 50 | 0.021612 | 0.011204 | 0.028190 |
| L7: C_rad/H/Cs\H2\Cs/O | | | | |
| L8: C_rad/H/Cs\H2\Cs—H2—Cs/O | | | | |
| L7: C_rad/H/Cs\H\Cs2/O | | | | |
| L6: C_rad/H/O2 | 2 | -0.016152 | 0.031780 | 0.015998 |
| L5: C_rad/H/OneDe | 185 | 0.086671 | -0.037595 | 0.049410 |
| L6: C_rad/H/OneDeC | 184 | 0.086442 | -0.037467 | 0.049316 |
| L7: C_rad/H/CtCs | | | | |
| L7: C_rad/H/CbCs | | | | |
| L7: C_rad/H/CO/Cs | 41 | 0.053933 | -0.014722 | 0.038508 |
| L8: C_rad/H/CO\H/Cs\H3 | 1 | 0.095705 | -0.050407 | 0.047214 |
| L7: C_rad/H/CdCs | 143 | 0.095805 | -0.044019 | 0.052429 |
| L7: C_rad/H/CSCs | | | | |
| L6: C_rad/H/OneDeO | 1 | 0.126124 | -0.059563 | 0.065670 |
| L5: C_rad/H/TwoDe | 99 | 0.126910 | -0.060266 | 0.068401 |

Continued on next page

**Table 1 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L6: C_rad/H/CtCt | | | | |
| L6: C_rad/H/CtCb | | | | |
| L6: C_rad/H/CtCO | | | | |
| L6: C_rad/H/CbCb | | | | |
| L6: C_rad/H/CbCO | | | | |
| L6: C_rad/H/COCO | | | | |
| L6: C_rad/H/CdCt | | | | |
| L6: C_rad/H/CdCb | | | | |
| L6: C_rad/H/CdCO | | | | |
| L6: C_rad/H/CdCd | 99 | 0.126910 | -0.060266 | 0.068401 |
| L4: C_ter_rad | 104 | 0.062942 | -0.025701 | 0.035402 |
| L5: C_rad/NonDe | 16 | 0.005813 | 0.000990 | 0.008314 |
| L6: C_rad/Cs3 | 15 | 0.007964 | 0.006028 | 0.015416 |
| L7: C_rad/Cs2/Cs\O | | | | |
| L7: C_rad/Cs3_5ring_fused6 | | | | |
| L7: C_rad/Cs3_5ring_adj5 | | | | |
| L6: C_rad/NDMustO | 1 | -0.049406 | -0.128339 | -0.173976 |
| L7: C_rad/Cs2O | 1 | -0.049406 | -0.128339 | -0.173976 |
| L8: C_rad/OOH/Cs/Cs | | | | |
| L8: C_rad/O/Cs/Cs\Cs | | | | |
| L7: C_rad/CsO2 | | | | |
| L7: C_rad/O3 | | | | |
| L5: C_rad/OneDe | 87 | 0.070669 | -0.029339 | 0.038898 |
| L6: C_rad/Cs2 | 87 | 0.070669 | -0.029339 | 0.038898 |
| L7: C_rad/CtCs2 | | | | |
| L7: C_rad/CbCs2 | | | | |
| L7: C_rad/COCs2 | 87 | 0.070669 | -0.029339 | 0.038898 |
| L7: C_rad/CdCs2 | | | | |
| L6: C_rad/CsO | | | | |
| L6: C_rad/O2 | | | | |
| L5: C_rad/TwoDe | 1 | 0.270660 | -0.119354 | 0.154191 |
| L6: C_rad/Cs | 1 | 0.270660 | -0.119354 | 0.154191 |
| L7: C_rad/CtCtCs | | | | |
| L7: C_rad/CtCbCs | | | | |
| L7: C_rad/CtCOCs | | | | |
| L7: C_rad/CbCbCs | | | | |
| L7: C_rad/CbCOCs | | | | |
| L7: C_rad/COCOCs | | | | |
| L7: C_rad/CdCtCs | | | | |
| L7: C_rad/CdCbCs | | | | |
| L7: C_rad/CdCOCs | | | | |
| L7: C_rad/CdCdCs | 1 | 0.270660 | -0.119354 | 0.154191 |
| L6: C_rad/TDMustO | | | | |
| L5: C_rad/ThreeDe | | | | |

## Group values for modified tree

Table 2: Modified tree structure, with distance group data in Å.

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L1: X_H_or_Xanyrad_H | 2142 | 1.335530 | 1.335350 | 2.666040 |
| L2: H2 | 70 | -0.342288 | -0.039783 | -0.379376 |
| L2: C_H | 1832 | 0.029362 | 0.004085 | 0.033720 |
| L3: Cs_H | 1304 | 0.013039 | 0.020558 | 0.034846 |
| L4: Csnorad_H | 1266 | 0.008578 | 0.024975 | 0.034745 |
| L5: C_methane | 69 | 0.076977 | -0.054808 | 0.025695 |
| L5: CsRHHH | 684 | 0.025708 | -0.000824 | 0.026630 |
| L6: CsCHHH | 631 | 0.025688 | -0.001134 | 0.026803 |
| L7: C/H3/Cs | 357 | 0.050417 | -0.030813 | 0.022318 |
| L7: C/H3/Cd | 154 | -0.016229 | 0.054933 | 0.041314 |
| L7: C/H3/Ct | 36 | -0.002891 | 0.027628 | 0.026874 |
| L7: C/H3/Cb | | | | |
| L6: CsOHHH | 53 | 0.025956 | 0.002967 | 0.024508 |
| L5: CsRRHH | 409 | -0.022947 | 0.070377 | 0.048092 |
| L6: CsCCHH | 356 | -0.028156 | 0.077681 | 0.050784 |
| L7: C/H2/Cs/Cs | 73 | 0.027797 | -0.011348 | 0.019668 |
| L7: C/H2/Cs/Cd | 143 | -0.039272 | 0.093747 | 0.055160 |
| L7: C/H2/Cs/Ct | | | | |
| L7: C/H2/Cs/Cb | | | | |
| L7: C/H2/Cd/Cd | 99 | -0.054862 | 0.123563 | 0.070441 |
| L7: C/H2/Cd/Ct | | | | |
| L7: C/H2/Cd/Cb | | | | |
| L7: C/H2/Ct/Ct | | | | |
| L7: C/H2/Ct/Cb | | | | |
| L7: C/H2/Cb/Cb | | | | |
| L6: CsCOHH | 51 | 0.011230 | 0.023228 | 0.030972 |
| L7: C/H2/Cs/O | 50 | 0.013016 | 0.020855 | 0.030315 |
| L7: C/H2/Cd/O | 1 | -0.064825 | 0.124233 | 0.058927 |
| L7: C/H2/Ct/O | | | | |
| L7: C/H2/Cb/O | | | | |
| L6: CsOOHH | 2 | 0.027312 | -0.019710 | 0.008337 |
| L5: CsRRRH | 104 | -0.024248 | 0.067372 | 0.041141 |
| L6: CsCCCH | 103 | -0.023913 | 0.067560 | 0.041645 |
| L7: C/H/Cs/Cs/Cs | 15 | 0.013473 | 0.013732 | 0.029444 |
| L7: C/H/Cs/Cs/Cd | | | | |
| L7: C/H/Cs/Cs/Ct | | | | |
| L7: C/H/Cs/Cs/Cb | | | | |
| L7: C/H/Cs/Cd/Cd | 1 | -0.121224 | 0.263641 | 0.145531 |
| L7: C/H/Cs/Cd/Ct | | | | |
| L7: C/H/Cs/Cd/Cb | | | | |
| L7: C/H/Cs/Ct/Ct | | | | |
| L7: C/H/Cs/Ct/Cb | | | | |
| L7: C/H/Cs/Cb/Cb | | | | |
| L7: C/H/Cd/Cd/Cd | | | | |
| L7: C/H/Cd/Cd/Ct | | | | |

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**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L7: C/H/Cd/Cd/Cb | | | | |
| L7: C/H/Cd/Ct/Ct | | | | |
| L7: C/H/Cd/Ct/Cb | | | | |
| L7: C/H/Cd/Cb/Cb | | | | |
| L7: C/H/Ct/Ct/Ct | | | | |
| L7: C/H/Ct/Ct/Cb | | | | |
| L7: C/H/Ct/Cb/Cb | | | | |
| L7: C/H/Cb/Cb/Cb | | | | |
| L6: CsCCOH | 1 | -0.121857 | 0.012401 | -0.106079 |
| L7: C/H/Cs/Cs/O | 1 | -0.121857 | 0.012401 | -0.106079 |
| L7: C/H/Cs/Cd/O | | | | |
| L7: C/H/Cs/Ct/O | | | | |
| L7: C/H/Cs/Cb/O | | | | |
| L7: C/H/Cd/Cd/O | | | | |
| L7: C/H/Cd/Ct/O | | | | |
| L7: C/H/Cd/Cb/O | | | | |
| L7: C/H/Ct/Ct/O | | | | |
| L7: C/H/Ct/Cb/O | | | | |
| L7: C/H/Cb/Cb/O | | | | |
| L6: CsCOOH | | | | |
| L7: C/H/Cs/O/O | | | | |
| L7: C/H/Cd/O/O | | | | |
| L7: C/H/Ct/O/O | | | | |
| L7: C/H/Cb/O/O | | | | |
| L6: CsOOOH | | | | |
| L4: Csrad_H | 38 | 0.154287 | -0.119281 | 0.038063 |
| L5: C_methyl | 38 | 0.154287 | -0.119281 | 0.038063 |
| L5: CsradRH2 | | | | |
| L6: CsradCHH | | | | |
| L7: Csrad/H/Cs/H | | | | |
| L7: Csrad/H/Cd/H | | | | |
| L7: Csrad/H/Ct/H | | | | |
| L7: Csrad/H/Cb/H | | | | |
| L6: CsradOH2 | | | | |
| L5: CsradRRH | | | | |
| L6: CsradCCH | | | | |
| L7: Csrad/Cs/Cs/H | | | | |
| L7: Csrad/Cs/Cd/H | | | | |
| L7: Csrad/Cs/Ct/H | | | | |
| L7: Csrad/Cs/Cb/H | | | | |
| L7: Csrad/Cd/Cd/H | | | | |
| L7: Csrad/Cd/Ct/H | | | | |
| L7: Csrad/Cd/Cb/H | | | | |
| L7: Csrad/Ct/Ct/H | | | | |
| L7: Csrad/Ct/Cb/H | | | | |
| L7: Csrad/Cb/Cb/H | | | | |
| L6: CsradCOH | | | | |
| L7: Csrad/Cs/O/H | | | | |

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**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L7: Csrad/Cd/O/H | | | | |
| L7: Csrad/Ct/O/H | | | | |
| L7: Csrad/Cb/O/H | | | | |
| L6: CsradOOH | | | | |
| L4: CsbiradH | | | | |
| L5: Cs_singletH | | | | |
| L6: Cs_singletHH | | | | |
| L6: Cs_singletRH | | | | |
| L7: C_singletCH | | | | |
| L8: C_singlet/Cs/H | | | | |
| L8: C_singlet/Cd/H | | | | |
| L8: C_singlet/Ct/H | | | | |
| L8: C_singlet/Cb/H | | | | |
| L7: C_singletOH | | | | |
| L5: Cs_tripletH | | | | |
| L6: Cs_tripletHH | | | | |
| L6: Cs_tripletRH | | | | |
| L7: Cs_tripletCH | | | | |
| L8: C_triplet/Cs/H | | | | |
| L8: C_triplet/Cd/H | | | | |
| L8: C_triplet/Ct/H | | | | |
| L8: C_triplet/Cb/H | | | | |
| L7: Cs_tripletOH | | | | |
| L4: CstriradH | | | | |
| L5: Cdoublet_H | | | | |
| L5: Cquartet_H | | | | |
| L3: Cd_H | 319 | 0.080461 | -0.066374 | 0.014535 |
| L4: Cdnorad_H | 319 | 0.080461 | -0.066374 | 0.014535 |
| L5: Cd_C/R/H | 319 | 0.080461 | -0.066374 | 0.014535 |
| L6: Cd_C/H2 | 210 | 0.075312 | -0.063805 | 0.011806 |
| L7: Cd_Cds/H2 | 121 | 0.112224 | -0.091421 | 0.021864 |
| L7: Cd_Cdd/H2 | 89 | 0.024935 | -0.026114 | -0.001921 |
| L6: Cd_C/C/H | 109 | 0.090623 | -0.071444 | 0.019920 |
| L7: Cd_Cds/Cs/H | 30 | 0.065391 | -0.049501 | 0.012283 |
| L7: Cd_Cds/Cd/H | 53 | 0.133020 | -0.104743 | 0.030985 |
| L7: Cd_Cds/Ct/H | 26 | 0.031752 | -0.027696 | 0.005788 |
| L7: Cd_Cds/Cb/H | | | | |
| L7: Cd_Cdd/Cs/H | | | | |
| L7: Cd_Cdd/Cd/H | | | | |
| L7: Cd_Cdd/Ct/H | | | | |
| L7: Cd_Cdd/Cb/H | | | | |
| L6: Cd_C/O/H | | | | |
| L7: Cd_Cds/O/H | | | | |
| L7: Cd_Cdd/O/H | | | | |
| L5: Cd_O/R/H | | | | |
| L6: Cd_O/H2 | | | | |
| L6: Cd_O/C/H | | | | |
| L7: Cd_O/Cs/H | | | | |

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**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L7: Cd_O/Cd/H | | | | |
| L7: Cd_O/Ct/H | | | | |
| L7: Cd_O/Cb/H | | | | |
| L6: Cd_O/O/H | | | | |
| L4: Cdrad_H | | | | |
| L5: Cdrad_C/H | | | | |
| L6: Cdrad_Cds/H | | | | |
| L6: Cdrad_Cdd/H | | | | |
| L5: Cdrad_O/H | | | | |
| L3: Ct_H | 12 | 0.431401 | -0.229422 | 0.108762 |
| L3: Cb_H | 44 | 0.117925 | -0.092504 | 0.026137 |
| L2: O_H | 240 | -0.118125 | -0.018878 | -0.139931 |
| L3: OradH | 15 | -0.075951 | -0.082791 | -0.155556 |
| L3: ORH | 225 | -0.121281 | -0.014095 | -0.138762 |
| L4: OHH | 14 | 0.070355 | -0.189952 | -0.151526 |
| L4: OCH | 52 | -0.066073 | -0.091363 | -0.160225 |
| L5: O/Cs/H | 51 | -0.064968 | -0.091454 | -0.159202 |
| L5: O/Cd/H | | | | |
| L5: O/Ct/H | | | | |
| L5: O/Cb/H | 1 | -0.234679 | -0.077629 | -0.316172 |
| L4: OOH | 159 | -0.156010 | 0.026510 | -0.130609 |
| L1: Y_anyrad | | | | |
| L2: Hrad | 70 | -0.039495 | -0.342287 | -0.379190 |
| L2: Orad | 240 | -0.017829 | -0.118668 | -0.139585 |
| L3: OjR | 225 | -0.012844 | -0.122031 | -0.138432 |
| L4: OjH | 14 | -0.193300 | 0.076164 | -0.149391 |
| L4: OjC | 52 | -0.089279 | -0.068097 | -0.160291 |
| L5: OjCs | 51 | -0.089356 | -0.066985 | -0.159249 |
| L5: OjCd | | | | |
| L5: OjCt | | | | |
| L5: OjCb | 1 | -0.077813 | -0.234351 | -0.316079 |
| L4: OjO | 159 | 0.027899 | -0.156949 | -0.130319 |
| L3: O_atom_triplet | 15 | -0.083286 | -0.074511 | -0.154718 |
| L2: Crad | 1832 | 0.003965 | 0.029654 | 0.033918 |
| L3: Cj | 1794 | 0.006693 | 0.026902 | 0.033836 |
| L4: Csj | 1266 | 0.025234 | 0.008380 | 0.034738 |
| L5: Cs_methyl | 69 | -0.053769 | 0.075442 | 0.025074 |
| L5: CsjRH2 | 684 | -0.000760 | 0.025831 | 0.026698 |
| L6: CsjCH2 | 631 | -0.001101 | 0.025831 | 0.026859 |
| L7: Csj/Cs/H2 | 357 | -0.031137 | 0.050803 | 0.022282 |
| L7: Csj/Cd/H2 | 154 | 0.055474 | -0.016532 | 0.041386 |
| L7: Csj/Ct/H2 | 36 | 0.028053 | -0.002911 | 0.027161 |
| L7: Csj/Cb/H2 | | | | |
| L6: CsjOH2 | 53 | 0.003401 | 0.025833 | 0.024741 |
| L5: CsjRRH | 409 | 0.070627 | -0.023160 | 0.048156 |
| L6: CsjCCH | 356 | 0.077902 | -0.028338 | 0.050848 |
| L7: Csj/Cs/Cs/H | 73 | -0.011458 | 0.028261 | 0.019955 |
| L7: Csj/Cs/Cd/H | 143 | 0.094158 | -0.039761 | 0.055281 |

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**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L7: Csj/Cs/Ct/H | | | | |
| L7: Csj/Cs/Cb/H | | | | |
| L7: Csj/Cd/Cd/H | 99 | 0.124292 | -0.055524 | 0.070403 |
| L7: Csj/Cd/Ct/H | | | | |
| L7: Csj/Cd/Cb/H | | | | |
| L7: Csj/Ct/Ct/H | | | | |
| L7: Csj/Ct/Cb/H | | | | |
| L7: Csj/Cb/Cb/H | | | | |
| L6: CsjCOH | 51 | 0.024012 | 0.010600 | 0.031199 |
| L7: Csj/Cs/O/H | 50 | 0.021572 | 0.012445 | 0.030539 |
| L7: Csj/Cd/O/H | 1 | 0.126136 | -0.066634 | 0.058822 |
| L7: Csj/Ct/O/H | | | | |
| L7: Csj/Cb/O/H | | | | |
| L6: CsjOOH | 2 | -0.017641 | 0.025276 | 0.008156 |
| L5: CsjRRR | 104 | 0.068516 | -0.025639 | 0.040796 |
| L6: CsjCCC | 103 | 0.068715 | -0.025301 | 0.041315 |
| L7: Csj/Cs/Cs/Cs | 15 | 0.013659 | 0.012220 | 0.028184 |
| L7: Csj/Cs/Cs/Cd | | | | |
| L7: Csj/Cs/Cs/Ct | | | | |
| L7: Csj/Cs/Cs/Cb | | | | |
| L7: Csj/Cs/Cd/Cd | 1 | 0.265941 | -0.123578 | 0.145242 |
| L7: Csj/Cs/Cd/Ct | | | | |
| L7: Csj/Cs/Cd/Cb | | | | |
| L7: Csj/Cs/Ct/Ct | | | | |
| L7: Csj/Cs/Ct/Cb | | | | |
| L7: Csj/Cs/Cb/Cb | | | | |
| L7: Csj/Cd/Cd/Cd | | | | |
| L7: Csj/Cd/Cd/Ct | | | | |
| L7: Csj/Cd/Cd/Cb | | | | |
| L7: Csj/Cd/Ct/Ct | | | | |
| L7: Csj/Cd/Ct/Cb | | | | |
| L7: Csj/Cd/Cb/Cb | | | | |
| L7: Csj/Ct/Ct/Ct | | | | |
| L7: Csj/Ct/Ct/Cb | | | | |
| L7: Csj/Ct/Cb/Cb | | | | |
| L7: Csj/Cb/Cb/Cb | | | | |
| L6: CsjCCO | 1 | 0.012218 | -0.121529 | -0.105986 |
| L7: Csj/Cs/Cs/O | 1 | 0.012218 | -0.121529 | -0.105986 |
| L7: Csj/Cs/Cd/O | | | | |
| L7: Csj/Cs/Ct/O | | | | |
| L7: Csj/Cs/Cb/O | | | | |
| L7: Csj/Cd/Cd/O | | | | |
| L7: Csj/Cd/Ct/O | | | | |
| L7: Csj/Cd/Cb/O | | | | |
| L7: Csj/Ct/Ct/O | | | | |
| L7: Csj/Ct/Cb/O | | | | |
| L7: Csj/Cb/Cb/O | | | | |
| L6: CsjCOO | | | | |

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**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L7: Csj/Cs/O/O | | | | |
| L7: Csj/Cd/O/O | | | | |
| L7: Csj/Ct/O/O | | | | |
| L7: Csj/Cb/O/O | | | | |
| L6: CsjOOO | | | | |
| L4: Cdj | 319 | -0.067745 | 0.082294 | 0.015358 |
| L5: Cdj_CR | 319 | -0.067745 | 0.082294 | 0.015358 |
| L6: Cdj_CH | 210 | -0.065277 | 0.077335 | 0.012609 |
| L7: Cdj_CdsH | 121 | -0.093854 | 0.115196 | 0.022945 |
| L7: Cdj_CddH | 89 | -0.026782 | 0.026331 | -0.001313 |
| L6: Cdj_CC | 109 | -0.072645 | 0.092142 | 0.020817 |
| L7: Cdj_CdsCs | 30 | -0.052748 | 0.067639 | 0.013440 |
| L7: Cdj_CdsCd | 53 | -0.104889 | 0.134137 | 0.031903 |
| L7: Cdj_CdsCt | 26 | -0.028231 | 0.032656 | 0.006171 |
| L7: Cdj_CdsCb | | | | |
| L7: Cdj_CddCs | | | | |
| L7: Cdj_CddCd | | | | |
| L7: Cdj_CddCt | | | | |
| L7: Cdj_CddCb | | | | |
| L6: Cdj_CO | | | | |
| L7: Cdj_CdsO | | | | |
| L7: Cdj_CddO | | | | |
| L5: Cdj_OR | | | | |
| L6: Cdj_OH | | | | |
| L6: Cdj_OC | | | | |
| L7: Cdj_OCs | | | | |
| L7: Cdj_OCd | | | | |
| L7: Cdj_OCt | | | | |
| L7: Cdj_OCb | | | | |
| L6: Cdj_OO | | | | |
| L4: Ctj | 12 | -0.230464 | 0.433568 | 0.110987 |
| L5: CtjC | 12 | -0.230464 | 0.433568 | 0.110987 |
| L4: Cbj | 44 | -0.095175 | 0.120179 | 0.026648 |
| L3: Cjj | 38 | -0.118072 | 0.152750 | 0.037583 |
| L4: Csjj | 38 | -0.118072 | 0.152750 | 0.037583 |
| L5: Cs_sing | | | | |
| L6: Cs_singH2 | | | | |
| L6: Cs_singRH | | | | |
| L7: Cs_singCH | | | | |
| L8: Cs_sing/Cs/H | | | | |
| L8: Cs_sing/Cd/H | | | | |
| L8: Cs_sing/Ct/H | | | | |
| L8: Cs_sing/Cb/H | | | | |
| L7: Cs_singOH | | | | |
| L6: Cs_singRR | | | | |
| L7: Cs_singCC | | | | |
| L8: Cs_sing/Cs/Cs | | | | |
| L8: Cs_sing/Cs/Cd | | | | |

Continued on next page

**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L8: Cs_sing/Cs/Ct | | | | |
| L8: Cs_sing/Cs/Cb | | | | |
| L8: Cs_sing/Cd/Cd | | | | |
| L8: Cs_sing/Cd/Ct | | | | |
| L8: Cs_sing/Cd/Cb | | | | |
| L8: Cs_sing/Ct/Ct | | | | |
| L8: Cs_sing/Ct/Cb | | | | |
| L8: Cs_sing/Cb/Cb | | | | |
| L7: Cs_singCO | | | | |
| L8: Cs_sing/Cs/O | | | | |
| L8: Cs_sing/Cd/O | | | | |
| L8: Cs_sing/Ct/O | | | | |
| L8: Cs_sing/Cb/O | | | | |
| L7: Cs_singOO | | | | |
| L5: Cs_trip | 38 | -0.118072 | 0.152750 | 0.037583 |
| L6: Cs_tripH2 | 38 | -0.118072 | 0.152750 | 0.037583 |
| L6: Cs_tripRH | | | | |
| L7: Cs_tripCH | | | | |
| L8: Cs_trip/Cs/H | | | | |
| L8: Cs_trip/Cd/H | | | | |
| L8: Cs_trip/Ct/H | | | | |
| L8: Cs_trip/Cb/H | | | | |
| L7: Cs_tripOH | | | | |
| L6: Cs_tripRR | | | | |
| L7: Cs_tripCC | | | | |
| L8: Cs_trip/Cs/Cs | | | | |
| L8: Cs_trip/Cs/Cd | | | | |
| L8: Cs_trip/Cs/Ct | | | | |
| L8: Cs_trip/Cs/Cb | | | | |
| L8: Cs_trip/Cd/Cd | | | | |
| L8: Cs_trip/Cd/Ct | | | | |
| L8: Cs_trip/Cd/Cb | | | | |
| L8: Cs_trip/Ct/Ct | | | | |
| L8: Cs_trip/Ct/Cb | | | | |
| L8: Cs_trip/Cb/Cb | | | | |
| L7: Cs_tripCO | | | | |
| L8: Cs_trip/Cs/O | | | | |
| L8: Cs_trip/Cd/O | | | | |
| L8: Cs_trip/Ct/O | | | | |
| L8: Cs_trip/Cb/O | | | | |
| L7: Cs_tripOO | | | | |
| L4: Cdjj | | | | |
| L5: Cd_singletR | | | | |
| L6: Cd_singletC | | | | |
| L6: Cd_singletO | | | | |
| L5: Cd_tripletR | | | | |
| L6: Cd_tripletC | | | | |
| L6: Cd_tripletO | | | | |

Continued on next page

**Table 2 – continued from previous page**

| Groups | TS count | dXH (Å) | dHY (Å) | dXY (Å) |
|---|---|---|---|---|
| L3: Cjjj | | | | |
| L4: C_doubletR | | | | |
| L4: C_quartetR | | | | |
| L3: Cjjjj | | | | |
| L4: C_quintet | | | | |
| L4: C_triplet | | | | |

## List of test reactions

Table 3: 1393 hydrogen abstraction reactions used to test the group estimates coupled with the automated transition state algorithm. The reactants and products are provided as SMILES strings. Transition states that were found and validated are available in CML format.

| Reactions | Found |
|---|---|
| [CH2]C(C)C(=O)C(C)C + [O]O ↔ CC(C)C(=O)C(C)C + [O][O] | No |
| C[C](C)C(=O)C(C)C + [O]O ↔ CC(C)C(=O)C(C)C + [O][O] | No |
| [CH2]C(C)C(=O)C(C)C + CC(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[C](C)C(=O)C(C)C | No |
| [CH2]C(C)C(=O)C(C)C + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)C + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C[C](C)C(=O)C(C)C + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)C + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C(C)C(=O)C(C)C + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)C + CC(C)C(=O)C(C)CO[O] | Yes |
| C[C](C)C(=O)C(C)C + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)C + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)C(=O)C(C)(C)O[O] + [O]O ↔ CC(C)C(=O)C(C)(C)OO + [O][O] | Yes |
| CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)CO[O] ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)CO[O] + [O]O ↔ CC(C)C(=O)C(C)COO + [O][O] | Yes |
| CC(C)C(=O)C(C)(C)OO + [H] ↔ [H][H] + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [H] ↔ [H][H] + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)C(=O)C(C)C + [O] ↔ [OH] + [CH2]C(C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)C + [O] ↔ [OH] + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [O] ↔ [OH] + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [O] ↔ [OH] + CC(C)C(=O)C(C)CO[O] | No |
| CC(C)C(=O)C(C)(C)OO + [OH] ↔ O + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [OH] ↔ O + CC(C)C(=O)C(C)CO[O] | No |
| CC(C)C(=O)C(C)(C)OO + [O]O ↔ OO + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [O]O ↔ OO + CC(C)C(=O)C(C)CO[O] | No |
| [CH2]C(C)C(=O)C(C)C + C#CC ↔ CC(C)C(=O)C(C)C + C#C[CH2] | No |
| CC(C)C(=O)C(C)C + C#C[CH2] ↔ C#CC + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)(C)OO + C#C[CH2] ↔ C#CC + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + C#C[CH2] ↔ C#CC + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + C#CC ↔ [H][H] + C#C[CH2] | Yes |
| [OH] + C#CC ↔ O + C#C[CH2] | Yes |
| [O]O + C#C[CH2] ↔ C#CC + [O][O] | No |
| OO + C#C[CH2] ↔ C#CC + [O]O | Yes |
| [CH2]C(C)C(=O)C(C)C + C=C=C ↔ CC(C)C(=O)C(C)C + [CH]=C=C | No |
| CC(C)C(=O)C(C)C + [CH]=C=C ↔ C=C=C + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C=C ↔ C=C=C + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [CH]=C=C ↔ C=C=C + CC(C)C(=O)C(C)CO[O] | No |
| [H] + C=C=C ↔ [H][H] + [CH]=C=C | No |
| [OH] + C=C=C ↔ O + [CH]=C=C | No |
| [O]O + [CH]=C=C ↔ C=C=C + [O][O] | No |
| OO + [CH]=C=C ↔ C=C=C + [O]O | No |
| [c]1ccccc1 + [O]O ↔ c1ccccc1 + [O][O] | No |
| [c]1ccccc1 + CC(C)C(=O)C(C)C ↔ c1ccccc1 + C[C](C)C(=O)C(C)C | No |
| [c]1ccccc1 + CC(C)C(=O)C(C)C ↔ c1ccccc1 + [CH2]C(C)C(=O)C(C)C | Yes |
| [c]1ccccc1 + CC(C)C(=O)C(C)(C)OO ↔ c1ccccc1 + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [c]1ccccc1 + CC(C)C(=O)C(C)COO ↔ c1ccccc1 + CC(C)C(=O)C(C)CO[O] | No |
| [c]1ccccc1 + [H][H] ↔ c1ccccc1 + [H] | Yes |

Continued on next page

**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| c1ccccc1 + [OH] ↔ O + [c]1ccccc1 | Yes |
| [c]1ccccc1 + OO ↔ c1ccccc1 + [O]O | No |
| [c]1ccccc1 + C#CC ↔ c1ccccc1 + C#C[CH2] | Yes |
| [c]1ccccc1 + C=C=C ↔ c1ccccc1 + [CH]=C=C | Yes |
| [CH2]C(C)C(=O)C(C)C + C=CC ↔ CC(C)C(=O)C(C)C + [CH2]C=C | No |
| C[C](C)C(=O)C(C)C + C=CC ↔ CC(C)C(=O)C(C)C + [CH2]C=C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2]C=C ↔ C=CC + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH2]C=C ↔ C=CC + CC(C)C(=O)C(C)CO[O] | Yes |
| OO + [CH2]C=C ↔ C=CC + [O]O | Yes |
| [c]1ccccc1 + C=CC ↔ c1ccccc1 + [CH2]C=C | No |
| C=C1C=C[CH]C1 + [O]O ↔ C=C1C=CCC1 + [O][O] | Yes |
| C=C1[CH]CC=C1 + [O]O ↔ C=C1C=CCC1 + [O][O] | Yes |
| C=C1C=CCC1 + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1[CH]CC=C1 | No |
| C=C1C=CCC1 + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1[CH]CC=C1 | Yes |
| C=C1C=CCC1 + CC(C)C(=O)C(C)(C)O[O] ↔ CC(C)C(=O)C(C)(C)OO + C=C1C=C[CH]C1 | Yes |
| C=C1[CH]CC=C1 + CC(C)C(=O)C(C)(C)OO ↔ C=C1C=CCC1 + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C=C1C=CCC1 + CC(C)C(=O)C(C)CO[O] ↔ CC(C)C(=O)C(C)COO + C=C1C=C[CH]C1 | Yes |
| C=C1[CH]CC=C1 + CC(C)C(=O)C(C)COO ↔ C=C1C=CCC1 + CC(C)C(=O)C(C)CO[O] | Yes |
| C=C1C=CCC1 + [H] ↔ [H][H] + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [H] ↔ [H][H] + C=C1[CH]CC=C1 | Yes |
| C=C1C=CCC1 + [O] ↔ [OH] + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [O] ↔ [OH] + C=C1[CH]CC=C1 | No |
| C=C1C=CCC1 + [OH] ↔ O + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + [OH] ↔ O + C=C1[CH]CC=C1 | No |
| C=C1C=CCC1 + [O]O ↔ OO + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + [O]O ↔ OO + C=C1[CH]CC=C1 | No |
| C=C1C=CCC1 + C#C[CH2] ↔ C#CC + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + C#C[CH2] ↔ C#CC + C=C1[CH]CC=C1 | Yes |
| C=C1C=CCC1 + [CH]=C=C ↔ C=C=C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH]=C=C ↔ C=C=C + C=C1[CH]CC=C1 | No |
| C=C1C=CCC1 + [c]1ccccc1 ↔ c1ccccc1 + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + [c]1ccccc1 ↔ c1ccccc1 + C=C1[CH]CC=C1 | Yes |
| C=C1C=CCC1 + [CH2]C=C ↔ C=CC + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH2]C=C ↔ C=CC + C=C1[CH]CC=C1 | Yes |
| C=C1[CH]C=CC1 + [O]O ↔ C=C1CC=CC1 + [O][O] | Yes |
| C=C1CC=CC1 + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1[CH]C=CC1 | Yes |
| C=C1CC=CC1 + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + CC(C)C(=O)C(C)(C)O[O] ↔ CC(C)C(=O)C(C)(C)OO + C=C1[CH]C=CC1 | Yes |
| C=C1CC=CC1 + CC(C)C(=O)C(C)CO[O] ↔ CC(C)C(=O)C(C)COO + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + [H] ↔ [H][H] + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + [O] ↔ [OH] + C=C1[CH]C=CC1 | Yes |
| C=C1CC=CC1 + [OH] ↔ O + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + [O]O ↔ OO + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + C#C[CH2] ↔ C#CC + C=C1[CH]C=CC1 | No |
| C=C1CC=CC1 + [CH]=C=C ↔ C=C=C + C=C1[CH]C=CC1 | Yes |
| C=C1CC=CC1 + [c]1ccccc1 ↔ c1ccccc1 + C=C1[CH]C=CC1 | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C1CC=CC1 + [CH2]C=C ↔ C=CC + C=C1[CH]C=CC1 | Yes |
| C=C1C=CCC1 + C=C1[CH]CC=C1 ↔ C=C1C=CCC1 + C=C1C=C[CH]C1 | No |
| C=C1CC=CC1 + C=C1[CH]CC=C1 ↔ C=C1C=CCC1 + C=C1[CH]C=CC1 | No |
| C=C1C=C[CH]C1 + C=C1CC=CC1 ↔ C=C1C=CCC1 + C=C1[CH]C=CC1 | No |
| CC(C)C(=O)C(C)C + [CH]=C ↔ C=C + [CH2]C(C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)C + [CH]=C ↔ C=C + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C ↔ C=C + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C ↔ C=C + CC(C)C(=O)C(C)CO[O] | No |
| [H][H] + [CH]=C ↔ C=C + [H] | Yes |
| [OH] + C=C ↔ O + [CH]=C | Yes |
| [O]O + [CH]=C ↔ C=C + [O][O] | Yes |
| OO + [CH]=C ↔ C=C + [O]O | No |
| [c]1ccccc1 + C=C ↔ c1ccccc1 + [CH]=C | No |
| C=C1C=CCC1 + [CH]=C ↔ C=C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH]=C ↔ C=C + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + [CH]=C ↔ C=C + C=C1[CH]C=CC1 | Yes |
| C=C=C + [O] ↔ [OH] + [CH]=C=C | Yes |
| C=C=C + C#C[CH2] ↔ C#CC + [CH]=C=C | Yes |
| [CH]=C=C + C=CC ↔ C=C=C + [CH2]C=C | No |
| C=C=C + [CH]=C ↔ C=C + [CH]=C=C | No |
| C#CC + [O] ↔ [OH] + C#C[CH2] | Yes |
| C#C[CH2] + C=CC ↔ C#CC + [CH2]C=C | Yes |
| C#CC + [CH]=C ↔ C=C + C#C[CH2] | No |
| [C]#C + [O]O ↔ C#C + [O][O] | Yes |
| [C]#C + CC(C)C(=O)C(C)C ↔ C#C + C[C](C)C(=O)C(C)C | No |
| [C]#C + CC(C)C(=O)C(C)C ↔ C#C + [CH2]C(C)C(=O)C(C)C | No |
| [C]#C + CC(C)C(=O)C(C)(C)OO ↔ C#C + CC(C)C(=O)C(C)(C)O[O] | No |
| [C]#C + CC(C)C(=O)C(C)COO ↔ C#C + CC(C)C(=O)C(C)CO[O] | No |
| [C]#C + [H][H] ↔ C#C + [H] | No |
| [C]#C + O ↔ C#C + [OH] | No |
| [C]#C + OO ↔ C#C + [O]O | No |
| [C]#C + C#CC ↔ C#C + C#C[CH2] | No |
| [C]#C + C=C=C ↔ C#C + [CH]=C=C | No |
| [C]#C + c1ccccc1 ↔ C#C + [c]1ccccc1 | No |
| [C]#C + C=CC ↔ C#C + [CH2]C=C | Yes |
| [C]#C + C=C1C=CCC1 ↔ C#C + C=C1[CH]CC=C1 | No |
| [C]#C + C=C1CC=CC1 ↔ C#C + C=C1[CH]C=CC1 | Yes |
| [C]#C + C=C1C=CCC1 ↔ C#C + C=C1C=C[CH]C1 | No |
| [C]#C + C=C ↔ C#C + [CH]=C | No |
| CC(C)C(=O)C(C)C + [CH]=CC ↔ C=CC + [CH2]C(C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)C + [CH]=CC ↔ C=CC + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC ↔ C=CC + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [CH]=CC ↔ C=CC + CC(C)C(=O)C(C)CO[O] | Yes |
| [O]O + [CH]=CC ↔ C=CC + [O][O] | No |
| OO + [CH]=CC ↔ C=CC + [O]O | No |
| [c]1ccccc1 + C=CC ↔ c1ccccc1 + [CH]=CC | No |
| C=C1C=CCC1 + [CH]=CC ↔ C=CC + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH]=CC ↔ C=CC + C=C1[CH]CC=C1 | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C1CC=CC1 + [CH]=CC ↔ C=CC + C=C1[CH]C=CC1 | No |
| C=C=C + [CH]=CC ↔ C=CC + [CH]=C=C | No |
| C#CC + [CH]=CC ↔ C=CC + C#C[CH2] | Yes |
| [C]#C + C=CC ↔ C#C + [CH]=CC | No |
| CC(C)C(=O)C(C)C + C=[C]C ↔ C=CC + [CH2]C(C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)C + C=[C]C ↔ C=CC + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + C=[C]C ↔ C=CC + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + C=[C]C ↔ C=CC + CC(C)C(=O)C(C)CO[O] | No |
| [O]O + C=[C]C ↔ C=CC + [O][O] | No |
| OO + C=[C]C ↔ C=CC + [O]O | No |
| [c]1ccccc1 + C=CC ↔ c1ccccc1 + C=[C]C | No |
| C=C1C=CCC1 + C=[C]C ↔ C=CC + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + C=[C]C ↔ C=CC + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + C=[C]C ↔ C=CC + C=C1[CH]C=CC1 | No |
| C=C=C + C=[C]C ↔ C=CC + [CH]=C=C | Yes |
| C#CC + C=[C]C ↔ C=CC + C#C[CH2] | Yes |
| [C]#C + C=CC ↔ C#C + C=[C]C | No |
| CC(C)C(=O)C(C)(C)OO + [CH3] ↔ C + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH3] ↔ C + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + C ↔ [H][H] + [CH3] | No |
| [OH] + C ↔ O + [CH3] | Yes |
| [O]O + [CH3] ↔ C + [O][O] | No |
| OO + [CH3] ↔ C + [O]O | No |
| [c]1ccccc1 + C ↔ c1ccccc1 + [CH3] | No |
| C=C1C=CCC1 + [CH3] ↔ C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH3] ↔ C + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + [CH3] ↔ C + C=C1[CH]C=CC1 | Yes |
| [C]#C + C ↔ C#C + [CH3] | Yes |
| CC(C)C(=O)C(C)C + [CH2]CC ↔ CCC + [CH2]C(C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)C + [CH2]CC ↔ CCC + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]CC ↔ CCC + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH2]CC ↔ CCC + CC(C)C(=O)C(C)CO[O] | Yes |
| OO + [CH2]CC ↔ CCC + [O]O | Yes |
| [c]1ccccc1 + CCC ↔ c1ccccc1 + [CH2]CC | No |
| C=C1C=CCC1 + [CH2]CC ↔ CCC + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH2]CC ↔ CCC + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + [CH2]CC ↔ CCC + C=C1[CH]C=CC1 | Yes |
| C=C=C + [CH2]CC ↔ CCC + [CH]=C=C | No |
| C#CC + [CH2]CC ↔ CCC + C#C[CH2] | Yes |
| [C]#C + CCC ↔ C#C + [CH2]CC | Yes |
| [CH2]C(C)C(=O)C(C)C + CCC ↔ CC(C)C(=O)C(C)C + C[CH]C | No |
| CC(C)C(=O)C(C)C + C[CH]C ↔ CCC + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + C[CH]C ↔ CCC + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + C[CH]C ↔ CCC + CC(C)C(=O)C(C)CO[O] | Yes |
| OO + C[CH]C ↔ CCC + [O]O | Yes |
| [c]1ccccc1 + CCC ↔ c1ccccc1 + C[CH]C | No |
| C=C1C=CCC1 + C[CH]C ↔ CCC + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + C[CH]C ↔ CCC + C=C1[CH]CC=C1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C1CC=CC1 + C[CH]C ↔ CCC + C=C1[CH]C=CC1 | Yes |
| C=C=C + C[CH]C ↔ CCC + [CH]=C=C | Yes |
| C#CC + C[CH]C ↔ CCC + C#C[CH2] | Yes |
| [C]#C + CCC ↔ C#C + C[CH]C | Yes |
| C=CC + [O] ↔ [OH] + [CH2]C=C | No |
| [CH]=CC + C=CC ↔ C=CC + [CH2]C=C | No |
| C=[C]C + C=CC ↔ C=CC + [CH2]C=C | No |
| [CH]=CC + C=C ↔ C=CC + [CH]=C | No |
| C=CC + [CH]=C ↔ C=C + C=[C]C | Yes |
| C=CC + [CH]=C ↔ C=C + [CH2]C=C | Yes |
| C=CC + [CH]=CC ↔ C=CC + C=[C]C | Yes |
| [CH]=CC + CCC ↔ C=CC + [CH2]CC | Yes |
| C=[C]C + CCC ↔ C=CC + [CH2]CC | Yes |
| C=CC + [CH2]CC ↔ CCC + [CH2]C=C | Yes |
| [CH]=CC + CCC ↔ C=CC + C[CH]C | Yes |
| C=[C]C + CCC ↔ C=CC + C[CH]C | Yes |
| C=CC + C[CH]C ↔ CCC + [CH2]C=C | Yes |
| [CH]=C + C ↔ C=C + [CH3] | Yes |
| [CH]=C + CCC ↔ C=C + [CH2]CC | Yes |
| [CH]=C + CCC ↔ C=C + C[CH]C | Yes |
| [CH]=C=O + [O]O ↔ C=C=O + [O][O] | Yes |
| [CH]=C=O + CC(C)C(=O)C(C)C ↔ C=C=O + C[C](C)C(=O)C(C)C | No |
| [CH]=C=O + CC(C)C(=O)C(C)C ↔ C=C=O + [CH2]C(C)C(=O)C(C)C | Yes |
| [CH]=C=O + CC(C)C(=O)C(C)(C)OO ↔ C=C=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH]=C=O + CC(C)C(=O)C(C)COO ↔ C=C=O + CC(C)C(=O)C(C)CO[O] | Yes |
| [CH]=C=O + [H][H] ↔ C=C=O + [H] | Yes |
| C=C=O + [OH] ↔ O + [CH]=C=O | Yes |
| [CH]=C=O + OO ↔ C=C=O + [O]O | Yes |
| [CH]=C=O + C#CC ↔ C=C=O + C#C[CH2] | Yes |
| [CH]=C=O + C=C=C ↔ C=C=O + [CH]=C=C | Yes |
| C=C=O + [c]1ccccc1 ↔ c1ccccc1 + [CH]=C=O | No |
| [CH]=C=O + C=CC ↔ C=C=O + [CH2]C=C | Yes |
| [CH]=C=O + C=C1C=CCC1 ↔ C=C=O + C=C1[CH]CC=C1 | Yes |
| [CH]=C=O + C=C1CC=CC1 ↔ C=C=O + C=C1[CH]C=CC1 | Yes |
| [CH]=C=O + C=C1C=CCC1 ↔ C=C=O + C=C1C=C[CH]C1 | Yes |
| C=C=O + [CH]=C ↔ C=C + [CH]=C=O | Yes |
| C=C=O + [CH]=CC ↔ C=CC + [CH]=C=O | Yes |
| C=C=O + C=[C]C ↔ C=CC + [CH]=C=O | Yes |
| [CH]=C=O + C ↔ C=C=O + [CH3] | Yes |
| [CH]=C=O + CCC ↔ C=C=O + [CH2]CC | Yes |
| [CH]=C=O + CCC ↔ C=C=O + C[CH]C | Yes |
| [CH]=O + [O]O ↔ C=O + [O][O] | Yes |
| C=O + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]=O | Yes |
| C=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]=O | Yes |
| [CH]=O + CC(C)C(=O)C(C)(C)OO ↔ C=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH]=O + CC(C)C(=O)C(C)COO ↔ C=O + CC(C)C(=O)C(C)CO[O] | Yes |
| C=O + [H] ↔ [H][H] + [CH]=O | Yes |
| C=O + [O] ↔ [OH] + [CH]=O | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=O + [OH] ↔ O + [CH]=O | No |
| [CH]=O + OO ↔ C=O + [O]O | No |
| C=O + C#C[CH2] ↔ C#CC + [CH]=O | Yes |
| C=O + [CH]=C=C ↔ C=C=C + [CH]=O | Yes |
| C=O + [c]1ccccc1 ↔ c1ccccc1 + [CH]=O | No |
| C=O + [CH2]C=C ↔ C=CC + [CH]=O | Yes |
| [CH]=O + C=C1C=CCC1 ↔ C=O + C=C1[CH]CC=C1 | Yes |
| [CH]=O + C=C1CC=CC1 ↔ C=O + C=C1[CH]C=CC1 | Yes |
| [CH]=O + C=C1C=CCC1 ↔ C=O + C=C1C=C[CH]C1 | Yes |
| C=O + [CH]=C ↔ C=C + [CH]=O | Yes |
| C=O + [CH]=CC ↔ C=CC + [CH]=O | Yes |
| C=O + C=[C]C ↔ C=CC + [CH]=O | Yes |
| C=O + [CH3] ↔ C + [CH]=O | Yes |
| C=O + [CH2]CC ↔ CCC + [CH]=O | Yes |
| C=O + C[CH]C ↔ CCC + [CH]=O | Yes |
| [CH2]O + [O]O ↔ CO + [O][O] | Yes |
| [CH2]O + CC(C)C(=O)C(C)C ↔ CO + C[C](C)C(=O)C(C)C | No |
| CO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]O | Yes |
| [CH2]O + CC(C)C(=O)C(C)(C)OO ↔ CO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]O + CC(C)C(=O)C(C)COO ↔ CO + CC(C)C(=O)C(C)CO[O] | Yes |
| CO + [H] ↔ [H][H] + [CH2]O | Yes |
| CO + [O] ↔ [OH] + [CH2]O | Yes |
| CO + [OH] ↔ O + [CH2]O | Yes |
| [CH2]O + C#CC ↔ CO + C#C[CH2] | No |
| [CH2]O + C=C=C ↔ CO + [CH]=C=C | Yes |
| CO + [c]1ccccc1 ↔ c1ccccc1 + [CH2]O | Yes |
| [CH2]O + C=CC ↔ CO + [CH2]C=C | Yes |
| [CH2]O + C=C1C=CCC1 ↔ CO + C=C1[CH]CC=C1 | Yes |
| [CH2]O + C=C1CC=CC1 ↔ CO + C=C1[CH]C=CC1 | Yes |
| [CH2]O + C=C1C=CCC1 ↔ CO + C=C1C=C[CH]C1 | Yes |
| CO + [CH]=C ↔ C=C + [CH2]O | Yes |
| CO + [CH]=CC ↔ C=CC + [CH2]O | Yes |
| CO + C=[C]C ↔ C=CC + [CH2]O | Yes |
| CO + [CH3] ↔ C + [CH2]O | Yes |
| CO + [CH2]CC ↔ CCC + [CH2]O | Yes |
| CO + C[CH]C ↔ CCC + [CH2]O | Yes |
| CC(C)C(=O)C(C)C + [CH2] ↔ [CH3] + [CH2]C(C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)C + [CH2] ↔ [CH3] + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2] ↔ [CH3] + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH2] ↔ [CH3] + CC(C)C(=O)C(C)CO[O] | Yes |
| [H][H] + [CH2] ↔ [CH3] + [H] | Yes |
| [O]O + [CH2] ↔ [CH3] + [O][O] | Yes |
| OO + [CH2] ↔ [CH3] + [O]O | No |
| C=C1C=CCC1 + [CH2] ↔ [CH3] + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + [CH2] ↔ [CH3] + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + [CH2] ↔ [CH3] + C=C1[CH]C=CC1 | Yes |
| C=C=C + [CH2] ↔ [CH3] + [CH]=C=C | Yes |
| C#CC + [CH2] ↔ [CH3] + C#C[CH2] | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=CC + [CH2] ↔ [CH3] + C=[C]C | Yes |
| C=CC + [CH2] ↔ [CH3] + [CH2]C=C | Yes |
| C=C + [CH2] ↔ [CH3] + [CH]=C | Yes |
| C=C=O + [CH2] ↔ [CH3] + [CH]=C=O | Yes |
| C=O + [CH2] ↔ [CH3] + [CH]=O | No |
| CO + [CH2] ↔ [CH3] + [CH2]O | Yes |
| C + [O] ↔ [OH] + [CH3] | No |
| C + [CH2] ↔ [CH3] + [CH3] | Yes |
| [CH2]CO + [O]O ↔ CCO + [O][O] | No |
| C[CH]O + [O]O ↔ CCO + [O][O] | No |
| CC[O] + [O]O ↔ CCO + [O][O] | No |
| [CH2]CO + CC(C)C(=O)C(C)C ↔ CCO + C[C](C)C(=O)C(C)C | No |
| C[CH]O + CC(C)C(=O)C(C)C ↔ CCO + C[C](C)C(=O)C(C)C | Yes |
| CC[O] + CC(C)C(=O)C(C)C ↔ CCO + C[C](C)C(=O)C(C)C | No |
| [CH2]CO + CC(C)C(=O)C(C)C ↔ CCO + [CH2]C(C)C(=O)C(C)C | No |
| CCO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[CH]O | Yes |
| CC[O] + CC(C)C(=O)C(C)C ↔ CCO + [CH2]C(C)C(=O)C(C)C | Yes |
| [CH2]CO + CC(C)C(=O)C(C)(C)OO ↔ CCO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C[CH]O + CC(C)C(=O)C(C)(C)OO ↔ CCO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC[O] + CC(C)C(=O)C(C)(C)OO ↔ CCO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]CO + CC(C)C(=O)C(C)COO ↔ CCO + CC(C)C(=O)C(C)CO[O] | No |
| C[CH]O + CC(C)C(=O)C(C)COO ↔ CCO + CC(C)C(=O)C(C)CO[O] | Yes |
| CC[O] + CC(C)C(=O)C(C)COO ↔ CCO + CC(C)C(=O)C(C)CO[O] | Yes |
| CCO + [O] ↔ [OH] + [CH2]CO | Yes |
| CCO + [O] ↔ [OH] + C[CH]O | Yes |
| CCO + [OH] ↔ O + [CH2]CO | No |
| CCO + [OH] ↔ O + CC[O] | No |
| [CH2]CO + OO ↔ CCO + [O]O | No |
| CC[O] + OO ↔ CCO + [O]O | Yes |
| [CH2]CO + C#CC ↔ CCO + C#C[CH2] | Yes |
| C[CH]O + C#CC ↔ CCO + C#C[CH2] | Yes |
| CC[O] + C#CC ↔ CCO + C#C[CH2] | Yes |
| [CH2]CO + C=C=C ↔ CCO + [CH]=C=C | Yes |
| C[CH]O + C=C=C ↔ CCO + [CH]=C=C | Yes |
| CC[O] + C=C=C ↔ CCO + [CH]=C=C | Yes |
| CCO + [c]1ccccc1 ↔ c1ccccc1 + [CH2]CO | Yes |
| CCO + [c]1ccccc1 ↔ c1ccccc1 + C[CH]O | Yes |
| CCO + [c]1ccccc1 ↔ c1ccccc1 + CC[O] | Yes |
| [CH2]CO + C=CC ↔ CCO + [CH2]C=C | No |
| C[CH]O + C=CC ↔ CCO + [CH2]C=C | Yes |
| CC[O] + C=CC ↔ CCO + [CH2]C=C | Yes |
| [CH2]CO + C=C1C=CCC1 ↔ CCO + C=C1[CH]CC=C1 | No |
| C[CH]O + C=C1C=CCC1 ↔ CCO + C=C1[CH]CC=C1 | Yes |
| CC[O] + C=C1C=CCC1 ↔ CCO + C=C1[CH]CC=C1 | Yes |
| [CH2]CO + C=C1CC=CC1 ↔ CCO + C=C1[CH]C=CC1 | No |
| C[CH]O + C=C1CC=CC1 ↔ CCO + C=C1[CH]C=CC1 | Yes |
| CC[O] + C=C1CC=CC1 ↔ CCO + C=C1[CH]C=CC1 | Yes |
| [CH2]CO + C=C1C=CCC1 ↔ CCO + C=C1C=C[CH]C1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C[CH]O + C=C1C=CCC1 ↔ CCO + C=C1C=C[CH]C1 | Yes |
| CC[O] + C=C1C=CCC1 ↔ CCO + C=C1C=C[CH]C1 | Yes |
| CCO + [CH]=C ↔ C=C + [CH2]CO | Yes |
| CCO + [CH]=C ↔ C=C + C[CH]O | Yes |
| CCO + [CH]=C ↔ C=C + CC[O] | No |
| CCO + [CH]=CC ↔ C=CC + [CH2]CO | Yes |
| CCO + [CH]=CC ↔ C=CC + C[CH]O | Yes |
| CCO + [CH]=CC ↔ C=CC + CC[O] | No |
| CCO + C=[C]C ↔ C=CC + [CH2]CO | No |
| CCO + C=[C]C ↔ C=CC + C[CH]O | Yes |
| CCO + C=[C]C ↔ C=CC + CC[O] | Yes |
| [CH2]CO + CCC ↔ CCO + [CH2]CC | No |
| CCO + [CH2]CC ↔ CCC + C[CH]O | Yes |
| CC[O] + CCC ↔ CCO + [CH2]CC | Yes |
| [CH2]CO + CCC ↔ CCO + C[CH]C | Yes |
| CCO + C[CH]C ↔ CCC + C[CH]O | Yes |
| CC[O] + CCC ↔ CCO + C[CH]C | Yes |
| CCO + [CH2] ↔ [CH3] + [CH2]CO | No |
| CCO + [CH2] ↔ [CH3] + C[CH]O | Yes |
| CCO + [CH2] ↔ [CH3] + CC[O] | Yes |
| [C]#C + CCO ↔ C#C + C[CH]O | No |
| [CH]=C=O + CCO ↔ C=C=O + C[CH]O | No |
| C=O + C[CH]O ↔ CCO + [CH]=O | No |
| [CH2]O + CCO ↔ CO + C[CH]O | Yes |
| [CH2]CO + CCO ↔ CCO + C[CH]O | Yes |
| CC[O] + CCO ↔ CCO + C[CH]O | Yes |
| [C]#C + CCO ↔ C#C + [CH2]CO | Yes |
| [CH]=C=O + CCO ↔ C=C=O + [CH2]CO | Yes |
| C=O + [CH2]CO ↔ CCO + [CH]=O | Yes |
| CO + [CH2]CO ↔ CCO + [CH2]O | Yes |
| CC[O] + CCO ↔ CCO + [CH2]CO | Yes |
| [C]#C + CCO ↔ C#C + CC[O] | Yes |
| [CH]=C=O + CCO ↔ C=C=O + CC[O] | No |
| C=O + CC[O] ↔ CCO + [CH]=O | Yes |
| CO + CC[O] ↔ CCO + [CH2]O | Yes |
| [CH2]C=O + CC(C)C(=O)C(C)C ↔ CC=O + C[C](C)C(=O)C(C)C | No |
| C[C]=O + CC(C)C(=O)C(C)C ↔ CC=O + C[C](C)C(=O)C(C)C | Yes |
| CC=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C=O | Yes |
| CC=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[C]=O | Yes |
| [CH2]C=O + CC(C)C(=O)C(C)(C)OO ↔ CC=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C[C]=O + CC(C)C(=O)C(C)(C)OO ↔ CC=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C=O + CC(C)C(=O)C(C)COO ↔ CC=O + CC(C)C(=O)C(C)CO[O] | Yes |
| C[C]=O + CC(C)C(=O)C(C)COO ↔ CC=O + CC(C)C(=O)C(C)CO[O] | Yes |
| CC=O + [H] ↔ [H][H] + [CH2]C=O | No |
| CC=O + [O] ↔ [OH] + [CH2]C=O | Yes |
| [CH2]C=O + C#CC ↔ CC=O + C#C[CH2] | Yes |
| CC=O + C#C[CH2] ↔ C#CC + C[C]=O | Yes |
| [CH2]C=O + C=C=C ↔ CC=O + [CH]=C=C | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC=O + [CH]=C=C ↔ C=C=C + C[C]=O | No |
| CC=O + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C=O | No |
| CC=O + [c]1ccccc1 ↔ c1ccccc1 + C[C]=O | Yes |
| [CH2]C=O + C=CC ↔ CC=O + [CH2]C=C | Yes |
| C[C]=O + C=CC ↔ CC=O + [CH2]C=C | Yes |
| [CH2]C=O + C=C1C=CCC1 ↔ CC=O + C=C1[CH]CC=C1 | Yes |
| C[C]=O + C=C1C=CCC1 ↔ CC=O + C=C1[CH]CC=C1 | Yes |
| [CH2]C=O + C=C1CC=CC1 ↔ CC=O + C=C1[CH]C=CC1 | Yes |
| C[C]=O + C=C1CC=CC1 ↔ CC=O + C=C1[CH]C=CC1 | Yes |
| [CH2]C=O + C=C1C=CCC1 ↔ CC=O + C=C1C=C[CH]C1 | Yes |
| C[C]=O + C=C1C=CCC1 ↔ CC=O + C=C1C=C[CH]C1 | Yes |
| CC=O + [CH]=C ↔ C=C + [CH2]C=O | Yes |
| CC=O + [CH]=C ↔ C=C + C[C]=O | No |
| CC=O + [CH]=CC ↔ C=CC + [CH2]C=O | Yes |
| CC=O + [CH]=CC ↔ C=CC + C[C]=O | Yes |
| CC=O + C=[C]C ↔ C=CC + [CH2]C=O | Yes |
| CC=O + C=[C]C ↔ C=CC + C[C]=O | Yes |
| CC=O + [CH2]CC ↔ CCC + [CH2]C=O | Yes |
| CC=O + [CH2]CC ↔ CCC + C[C]=O | Yes |
| CC=O + C[CH]C ↔ CCC + [CH2]C=O | Yes |
| CC=O + C[CH]C ↔ CCC + C[C]=O | Yes |
| CC=O + [CH2] ↔ [CH3] + [CH2]C=O | Yes |
| CC=O + [CH2] ↔ [CH3] + C[C]=O | Yes |
| [CH2]C=O + CCO ↔ CC=O + C[CH]O | No |
| CC=O + C[CH]O ↔ CCO + C[C]=O | Yes |
| CC=O + [CH2]CO ↔ CCO + [CH2]C=O | Yes |
| CC=O + [CH2]CO ↔ CCO + C[C]=O | Yes |
| CC=O + CC[O] ↔ CCO + [CH2]C=O | Yes |
| CC=O + CC[O] ↔ CCO + C[C]=O | Yes |
| [C]#C + CC=O ↔ C#C + C[C]=O | Yes |
| [CH]=C=O + CC=O ↔ C=C=O + C[C]=O | No |
| C=O + C[C]=O ↔ CC=O + [CH]=O | No |
| [CH2]O + CC=O ↔ CO + C[C]=O | Yes |
| [CH2]C=O + CC=O ↔ CC=O + C[C]=O | Yes |
| [C]#C + CC=O ↔ C#C + [CH2]C=O | Yes |
| [CH]=C=O + CC=O ↔ C=C=O + [CH2]C=O | No |
| C=O + [CH2]C=O ↔ CC=O + [CH]=O | Yes |
| CO + [CH2]C=O ↔ CC=O + [CH2]O | Yes |
| [CH2]C(C)C(=O)C(C)C + CC ↔ CC(C)C(=O)C(C)C + C[CH2] | Yes |
| CC(C)C(=O)C(C)C + C[CH2] ↔ CC + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + C[CH2] ↔ CC + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + C[CH2] ↔ CC + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + CC ↔ [H][H] + C[CH2] | Yes |
| [OH] + CC ↔ O + C[CH2] | Yes |
| OO + C[CH2] ↔ CC + [O]O | No |
| [c]1ccccc1 + CC ↔ c1ccccc1 + C[CH2] | No |
| C=C1C=CCC1 + C[CH2] ↔ CC + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + C[CH2] ↔ CC + C=C1[CH]CC=C1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C1CC=CC1 + C[CH2] ↔ CC + C=C1[CH]C=CC1 | Yes |
| C=C=C + C[CH2] ↔ CC + [CH]=C=C | Yes |
| C#CC + C[CH2] ↔ CC + C#C[CH2] | Yes |
| [C]#C + CC ↔ C#C + C[CH2] | Yes |
| [CH]=CC + CC ↔ C=CC + C[CH2] | No |
| C=[C]C + CC ↔ C=CC + C[CH2] | Yes |
| C=CC + C[CH2] ↔ CC + [CH2]C=C | Yes |
| [CH]=C + CC ↔ C=C + C[CH2] | Yes |
| [CH]=C=O + CC ↔ C=C=O + C[CH2] | Yes |
| C=O + C[CH2] ↔ CC + [CH]=O | No |
| CO + C[CH2] ↔ CC + [CH2]O | Yes |
| [CH3] + CC ↔ C + C[CH2] | Yes |
| [CH2]CO + CC ↔ CCO + C[CH2] | Yes |
| CCO + C[CH2] ↔ CC + C[CH]O | Yes |
| CC[O] + CC ↔ CCO + C[CH2] | Yes |
| CC=O + C[CH2] ↔ CC + [CH2]C=O | Yes |
| CC=O + C[CH2] ↔ CC + C[C]=O | Yes |
| CC + [O] ↔ [OH] + C[CH2] | Yes |
| CC + [CH2]CC ↔ CCC + C[CH2] | Yes |
| C[CH2] + CCC ↔ CC + C[CH]C | Yes |
| CC + [CH2] ↔ [CH3] + C[CH2] | Yes |
| [C]#C + C=C=O ↔ C#C + [CH]=C=O | Yes |
| C=O + [CH]=C=O ↔ C=C=O + [CH]=O | No |
| CO + [CH]=C=O ↔ C=C=O + [CH2]O | Yes |
| [C]#C + CO ↔ C#C + [CH2]O | No |
| C=O + [CH2]O ↔ CO + [CH]=O | No |
| C=O + [C]#C ↔ C#C + [CH]=O | No |
| CCC + [O] ↔ [OH] + [CH2]CC | No |
| CCC + [O] ↔ [OH] + C[CH]C | Yes |
| CCC + [CH2]CC ↔ CCC + C[CH]C | Yes |
| CCC + [CH2] ↔ [CH3] + [CH2]CC | Yes |
| CCC + [CH2] ↔ [CH3] + C[CH]C | Yes |
| [CH2]C=C=O + [O]O ↔ CC=C=O + [O][O] | Yes |
| [CH2]C=C=O + CC(C)C(=O)C(C)C ↔ CC=C=O + C[C](C)C(=O)C(C)C | Yes |
| CC=C=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C=C=O | Yes |
| [CH2]C=C=O + CC(C)C(=O)C(C)(C)OO ↔ CC=C=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C=C=O + CC(C)C(=O)C(C)COO ↔ CC=C=O + CC(C)C(=O)C(C)CO[O] | Yes |
| [CH2]C=C=O + OO ↔ CC=C=O + [O]O | Yes |
| CC=C=O + C#C[CH2] ↔ C#CC + [CH2]C=C=O | Yes |
| [CH2]C=C=O + C=C=C ↔ CC=C=O + [CH]=C=C | Yes |
| CC=C=O + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C=C=O | Yes |
| [CH2]C=C=O + C=CC ↔ CC=C=O + [CH2]C=C | Yes |
| [CH2]C=C=O + C=C1C=CCC1 ↔ CC=C=O + C=C1[CH]CC=C1 | Yes |
| [CH2]C=C=O + C=C1CC=CC1 ↔ CC=C=O + C=C1[CH]C=CC1 | Yes |
| [CH2]C=C=O + C=C1C=CCC1 ↔ CC=C=O + C=C1C=C[CH]C1 | Yes |
| CC=C=O + [CH]=C ↔ C=C + [CH2]C=C=O | Yes |
| CC=C=O + [CH]=CC ↔ C=CC + [CH2]C=C=O | No |
| CC=C=O + C=[C]C ↔ C=CC + [CH2]C=C=O | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC=C=O + [CH3] ↔ C + [CH2]C=C=O | Yes |
| CC=C=O + [CH2]CC ↔ CCC + [CH2]C=C=O | No |
| CC=C=O + C[CH]C ↔ CCC + [CH2]C=C=O | Yes |
| CC=C=O + [CH2] ↔ [CH3] + [CH2]C=C=O | Yes |
| CC=C=O + C[CH]O ↔ CCO + [CH2]C=C=O | No |
| CC=C=O + [CH2]CO ↔ CCO + [CH2]C=C=O | Yes |
| CC=C=O + CC[O] ↔ CCO + [CH2]C=C=O | Yes |
| [CH2]C=C=O + CC=O ↔ CC=C=O + C[C]=O | No |
| CC=C=O + [CH2]C=O ↔ CC=O + [CH2]C=C=O | Yes |
| CC=C=O + C[CH2] ↔ CC + [CH2]C=C=O | Yes |
| CC=C=O + [CH]=C=O ↔ C=C=O + [CH2]C=C=O | Yes |
| CC=C=O + [CH2]O ↔ CO + [CH2]C=C=O | No |
| CC=C=O + [C]#C ↔ C#C + [CH2]C=C=O | Yes |
| [CH2]C=C=O + C=O ↔ CC=C=O + [CH]=O | No |
| [CH2]C(C)C(=O)C(C)C + C=CC=O ↔ CC(C)C(=O)C(C)C + C=C[C]=O | No |
| CC(C)C(=O)C(C)C + C=C[C]=O ↔ C=CC=O + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + C=C[C]=O ↔ C=CC=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + C=C[C]=O ↔ C=CC=O + CC(C)C(=O)C(C)CO[O] | Yes |
| OO + C=C[C]=O ↔ C=CC=O + [O]O | Yes |
| [c]1ccccc1 + C=CC=O ↔ c1ccccc1 + C=C[C]=O | No |
| C=C1C=CCC1 + C=C[C]=O ↔ C=CC=O + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + C=C[C]=O ↔ C=CC=O + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + C=C[C]=O ↔ C=CC=O + C=C1[CH]C=CC1 | Yes |
| [CH]=C=C + C=CC=O ↔ C=C=C + C=C[C]=O | Yes |
| C#C[CH2] + C=CC=O ↔ C#CC + C=C[C]=O | No |
| [C]#C + C=CC=O ↔ C#C + C=C[C]=O | No |
| [CH]=CC + C=CC=O ↔ C=CC + C=C[C]=O | No |
| C=[C]C + C=CC=O ↔ C=CC + C=C[C]=O | No |
| C=CC + C=C[C]=O ↔ C=CC=O + [CH2]C=C | Yes |
| [CH]=C + C=CC=O ↔ C=C + C=C[C]=O | Yes |
| [CH]=C=O + C=CC=O ↔ C=C=O + C=C[C]=O | No |
| C=O + C=C[C]=O ↔ C=CC=O + [CH]=O | Yes |
| [CH2]O + C=CC=O ↔ CO + C=C[C]=O | Yes |
| [CH3] + C=CC=O ↔ C + C=C[C]=O | Yes |
| [CH2]CO + C=CC=O ↔ CCO + C=C[C]=O | Yes |
| C[CH]O + C=CC=O ↔ CCO + C=C[C]=O | Yes |
| CC[O] + C=CC=O ↔ CCO + C=C[C]=O | Yes |
| [CH2]C=O + C=CC=O ↔ CC=O + C=C[C]=O | Yes |
| CC=O + C=C[C]=O ↔ C=CC=O + C[C]=O | Yes |
| C[CH2] + C=CC=O ↔ CC + C=C[C]=O | Yes |
| [CH2]CC + C=CC=O ↔ CCC + C=C[C]=O | No |
| C[CH]C + C=CC=O ↔ CCC + C=C[C]=O | Yes |
| [CH2]C=C=O + C=CC=O ↔ CC=C=O + C=C[C]=O | Yes |
| C=CC=O + [CH2] ↔ [CH3] + C=C[C]=O | Yes |
| CC(C)C(=O)C(C)C + [CH]=CC#C ↔ C#CC=C + [CH2]C(C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)C + [CH]=CC#C ↔ C#CC=C + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC#C ↔ C#CC=C + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + [CH]=CC#C ↔ C#CC=C + CC(C)C(=O)C(C)CO[O] | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| [H][H] + [CH]=CC#C ↔ C#CC=C + [H] | Yes |
| [OH] + C#CC=C ↔ O + [CH]=CC#C | Yes |
| [O]O + [CH]=CC#C ↔ C#CC=C + [O][O] | No |
| OO + [CH]=CC#C ↔ C#CC=C + [O]O | No |
| c1ccccc1 + [CH]=CC#C ↔ C#CC=C + [c]1ccccc1 | No |
| C=C1C=CCC1 + [CH]=CC#C ↔ C#CC=C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + [CH]=CC#C ↔ C#CC=C + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + [CH]=CC#C ↔ C#CC=C + C=C1[CH]C=CC1 | No |
| C=C=C + [CH]=CC#C ↔ C#CC=C + [CH]=C=C | Yes |
| C#CC + [CH]=CC#C ↔ C#CC=C + C#C[CH2] | Yes |
| [C]#C + C#CC=C ↔ C#C + [CH]=CC#C | Yes |
| C=CC + [CH]=CC#C ↔ C#CC=C + [CH]=CC | Yes |
| C=CC + [CH]=CC#C ↔ C#CC=C + C=[C]C | Yes |
| C=CC + [CH]=CC#C ↔ C#CC=C + [CH2]C=C | Yes |
| C=C + [CH]=CC#C ↔ C#CC=C + [CH]=C | No |
| C=C=O + [CH]=CC#C ↔ C#CC=C + [CH]=C=O | Yes |
| C=O + [CH]=CC#C ↔ C#CC=C + [CH]=O | Yes |
| CO + [CH]=CC#C ↔ C#CC=C + [CH2]O | No |
| C + [CH]=CC#C ↔ C#CC=C + [CH3] | No |
| CCO + [CH]=CC#C ↔ C#CC=C + [CH2]CO | Yes |
| CCO + [CH]=CC#C ↔ C#CC=C + C[CH]O | Yes |
| CCO + [CH]=CC#C ↔ C#CC=C + CC[O] | Yes |
| CC=O + [CH]=CC#C ↔ C#CC=C + [CH2]C=O | Yes |
| CC=O + [CH]=CC#C ↔ C#CC=C + C[C]=O | Yes |
| CC + [CH]=CC#C ↔ C#CC=C + C[CH2] | Yes |
| CCC + [CH]=CC#C ↔ C#CC=C + [CH2]CC | No |
| CCC + [CH]=CC#C ↔ C#CC=C + C[CH]C | Yes |
| CC=C=O + [CH]=CC#C ↔ C#CC=C + [CH2]C=C=O | Yes |
| C=CC=O + [CH]=CC#C ↔ C#CC=C + C=C[C]=O | Yes |
| CC(C)C(=O)C(C)C + C#C[C]=C ↔ C#CC=C + [CH2]C(C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)C + C#C[C]=C ↔ C#CC=C + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + C#C[C]=C ↔ C#CC=C + CC(C)C(=O)C(C)(C)O[O] | No |
| CC(C)C(=O)C(C)COO + C#C[C]=C ↔ C#CC=C + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + C#CC=C ↔ [H][H] + C#C[C]=C | Yes |
| [OH] + C#CC=C ↔ O + C#C[C]=C | Yes |
| [O]O + C#C[C]=C ↔ C#CC=C + [O][O] | No |
| OO + C#C[C]=C ↔ C#CC=C + [O]O | No |
| [c]1ccccc1 + C#CC=C ↔ c1ccccc1 + C#C[C]=C | No |
| C=C1C=CCC1 + C#C[C]=C ↔ C#CC=C + C=C1C=C[CH]C1 | Yes |
| C=C1C=CCC1 + C#C[C]=C ↔ C#CC=C + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + C#C[C]=C ↔ C#CC=C + C=C1[CH]C=CC1 | Yes |
| C=C=C + C#C[C]=C ↔ C#CC=C + [CH]=C=C | Yes |
| C#CC + C#C[C]=C ↔ C#CC=C + C#C[CH2] | No |
| [C]#C + C#CC=C ↔ C#C + C#C[C]=C | No |
| [CH]=CC + C#CC=C ↔ C=CC + C#C[C]=C | No |
| C=[C]C + C#CC=C ↔ C=CC + C#C[C]=C | No |
| C=CC + C#C[C]=C ↔ C#CC=C + [CH2]C=C | Yes |
| [CH]=C + C#CC=C ↔ C=C + C#C[C]=C | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| [CH]=C=O + C#CC=C ↔ C=C=O + C#C[C]=C | Yes |
| C=O + C#C[C]=C ↔ C#CC=C + [CH]=O | Yes |
| CO + C#C[C]=C ↔ C#CC=C + [CH2]O | Yes |
| [CH3] + C#CC=C ↔ C + C#C[C]=C | Yes |
| [CH2]CO + C#CC=C ↔ CCO + C#C[C]=C | No |
| CCO + C#C[C]=C ↔ C#CC=C + C[CH]O | No |
| CC[O] + C#CC=C ↔ CCO + C#C[C]=C | Yes |
| CC=O + C#C[C]=C ↔ C#CC=C + [CH2]C=O | Yes |
| CC=O + C#C[C]=C ↔ C#CC=C + C[C]=O | Yes |
| CC + C#C[C]=C ↔ C#CC=C + C[CH2] | Yes |
| CCC + C#C[C]=C ↔ C#CC=C + [CH2]CC | No |
| CCC + C#C[C]=C ↔ C#CC=C + C[CH]C | Yes |
| CC=C=O + C#C[C]=C ↔ C#CC=C + [CH2]C=C=O | Yes |
| C=CC=O + C#C[C]=C ↔ C#CC=C + C=C[C]=O | No |
| C#CC=C + [O] ↔ [OH] + C#C[C]=C | Yes |
| C#CC=C + [CH2] ↔ [CH3] + C#C[C]=C | Yes |
| C#CC=C + [CH]=CC#C ↔ C#CC=C + C#C[C]=C | Yes |
| C[C](C)C(=O)C(C)(C)OO + [O]O ↔ CC(C)C(=O)C(C)(C)OO + [O][O] | Yes |
| C[C](C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)(C)OO + C[C](C)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[C](C)C(=O)C(C)(C)OO | Yes |
| C[C](C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C[C](C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)CO[O] | No |
| CC(C)C(=O)C(C)(C)OO + [H] ↔ [H][H] + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [O] ↔ [OH] + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [OH] ↔ O + C[C](C)C(=O)C(C)(C)OO | No |
| C[C](C)C(=O)C(C)(C)OO + OO ↔ CC(C)C(=O)C(C)(C)OO + [O]O | No |
| CC(C)C(=O)C(C)(C)OO + C#C[CH2] ↔ C#CC + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C=C ↔ C=C=C + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [c]1ccccc1 ↔ c1ccccc1 + C[C](C)C(=O)C(C)(C)OO | No |
| C[C](C)C(=O)C(C)(C)OO + C=CC ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C=C | No |
| C[C](C)C(=O)C(C)(C)OO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1[CH]CC=C1 | Yes |
| C[C](C)C(=O)C(C)(C)OO + C=C1CC=CC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1[CH]C=CC1 | Yes |
| C[C](C)C(=O)C(C)(C)OO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1C=C[CH]C1 | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C ↔ C=C + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC ↔ C=CC + C[C](C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + C=[C]C ↔ C=CC + C[C](C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + [CH3] ↔ C + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2]CC ↔ CCC + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + C[CH]C ↔ CCC + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2] ↔ [CH3] + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + C[CH]O ↔ CCO + C[C](C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]CO ↔ CCO + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + CC[O] ↔ CCO + C[C](C)C(=O)C(C)(C)OO | Yes |
| C[C](C)C(=O)C(C)(C)OO + CC=O ↔ CC(C)C(=O)C(C)(C)OO + C[C]=O | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]C=O ↔ CC=O + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + C[CH2] ↔ CC + C[C](C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + [CH]=C=O ↔ C=C=O + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2]O ↔ CO + C[C](C)C(=O)C(C)(C)OO | No |

Continued on next page

**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC(C)C(=O)C(C)(C)OO + [C]#C ↔ C#C + C[C](C)C(=O)C(C)(C)OO | Yes |
| C[C](C)C(=O)C(C)(C)OO + C=O ↔ CC(C)C(=O)C(C)(C)OO + [CH]=O | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]C=C=O ↔ CC=C=O + C[C](C)C(=O)C(C)(C)OO | No |
| C[C](C)C(=O)C(C)(C)OO + C=CC=O ↔ CC(C)C(=O)C(C)(C)OO + C=C[C]=O | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC#C ↔ C#CC=C + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + C#C[C]=C ↔ C#CC=C + C[C](C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + [O]O ↔ CC(C)C(=O)C(C)(C)OO + [O][O] | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)(C)OO + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)C(=O)C(C)(C)OO + [H] ↔ [H][H] + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [O] ↔ [OH] + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [OH] ↔ O + [CH2]C(C)C(=O)C(C)(C)OO | No |
| [CH2]C(C)C(=O)C(C)(C)OO + OO ↔ CC(C)C(=O)C(C)(C)OO + [O]O | No |
| [CH2]C(C)C(=O)C(C)(C)OO + C#CC ↔ CC(C)C(=O)C(C)(C)OO + C#C[CH2] | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + C=C=C ↔ CC(C)C(=O)C(C)(C)OO + [CH]=C=C | Yes |
| CC(C)C(=O)C(C)(C)OO + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + C=CC ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C=C | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1[CH]CC=C1 | No |
| [CH2]C(C)C(=O)C(C)(C)OO + C=C1CC=CC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1[CH]C=CC1 | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)(C)OO + C=C1C=C[CH]C1 | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C ↔ C=C + [CH2]C(C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC ↔ C=CC + [CH2]C(C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + C=[C]C ↔ C=CC + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH3] ↔ C + [CH2]C(C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]CC ↔ CCC + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CCC ↔ CC(C)C(=O)C(C)(C)OO + C[CH]C | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH2] ↔ [CH3] + [CH2]C(C)C(=O)C(C)(C)OO | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CCO ↔ CC(C)C(=O)C(C)(C)OO + C[CH]O | No |
| CC(C)C(=O)C(C)(C)OO + [CH2]CO ↔ CCO + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| CC(C)C(=O)C(C)(C)OO + CC[O] ↔ CCO + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CC=O ↔ CC(C)C(=O)C(C)(C)OO + C[C]=O | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CC=O ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C=O | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CC ↔ CC(C)C(=O)C(C)(C)OO + C[CH2] | Yes |
| CC(C)C(=O)C(C)(C)OO + [CH]=C=O ↔ C=C=O + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CO ↔ CC(C)C(=O)C(C)(C)OO + [CH2]O | Yes |
| CC(C)C(=O)C(C)(C)OO + [C]#C ↔ C#C + [CH2]C(C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + C=O ↔ CC(C)C(=O)C(C)(C)OO + [CH]=O | Yes |
| [CH2]C(C)C(=O)C(C)(C)OO + CC=C=O ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C=C=O | No |
| [CH2]C(C)C(=O)C(C)(C)OO + C=CC=O ↔ CC(C)C(=O)C(C)(C)OO + C=C[C]=O | No |
| CC(C)C(=O)C(C)(C)OO + [CH]=CC#C ↔ C#CC=C + [CH2]C(C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + C#C[C]=C ↔ C#CC=C + [CH2]C(C)C(=O)C(C)(C)OO | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + C[C](C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(C)C(=O)C(C)C + CC(C)C(=O)OO ↔ CC(C)C(=O)C(C)C + CC(C)C(=O)O[O] | Yes |
| CC(C)C(=O)C(C)C + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[C](C)C(=O)C(C)C | No |
| [CH2]C(C)C(=O)C(C)(C)OO + CC(C)C(=O)OO ↔ CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)O[O] | Yes |
| CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[C](C)C(=O)C(C)(C)OO | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC(C)C(=O)C(C)(C)OO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + CC(C)C(=O)OO ↔ [H][H] + CC(C)C(=O)O[O] | Yes |
| [OH] + CC(C)C(=O)OO ↔ O + CC(C)C(=O)O[O] | No |
| [O]O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [O][O] | No |
| OO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [O]O | No |
| [c]1ccccc1 + CC(C)C(=O)OO ↔ c1ccccc1 + CC(C)C(=O)O[O] | No |
| C=C1C=CCC1 + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C=C1[CH]C=CC1 | Yes |
| C=C=C + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH]=C=C | No |
| C#CC + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C#C[CH2] | Yes |
| [C]#C + CC(C)C(=O)OO ↔ C#C + CC(C)C(=O)O[O] | No |
| [CH]=CC + CC(C)C(=O)OO ↔ C=CC + CC(C)C(=O)O[O] | No |
| C=[C]C + CC(C)C(=O)OO ↔ C=CC + CC(C)C(=O)O[O] | No |
| C=CC + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]C=C | No |
| [CH]=C + CC(C)C(=O)OO ↔ C=C + CC(C)C(=O)O[O] | Yes |
| [CH]=C=O + CC(C)C(=O)OO ↔ C=C=O + CC(C)C(=O)O[O] | No |
| C=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH]=O | No |
| CO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]O | No |
| [CH3] + CC(C)C(=O)OO ↔ C + CC(C)C(=O)O[O] | No |
| [CH2]CO + CC(C)C(=O)OO ↔ CCO + CC(C)C(=O)O[O] | No |
| CCO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[CH]O | No |
| CC[O] + CC(C)C(=O)OO ↔ CCO + CC(C)C(=O)O[O] | Yes |
| CC=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]C=O | Yes |
| CC=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[C]=O | Yes |
| C[CH2] + CC(C)C(=O)OO ↔ CC + CC(C)C(=O)O[O] | Yes |
| [CH2]CC + CC(C)C(=O)OO ↔ CCC + CC(C)C(=O)O[O] | No |
| CCC + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[CH]C | No |
| CC=C=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]C=C=O | No |
| C=CC=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C=C[C]=O | No |
| C#C[C]=C + CC(C)C(=O)OO ↔ C#CC=C + CC(C)C(=O)O[O] | No |
| [CH]=CC#C + CC(C)C(=O)OO ↔ C#CC=C + CC(C)C(=O)O[O] | No |
| CC(C)C(=O)OO + [CH2] ↔ [CH3] + CC(C)C(=O)O[O] | No |
| C[C](C)C(=O)C(C)COO + [O]O ↔ CC(C)C(=O)C(C)COO + [O][O] | Yes |
| C[C](C)C(=O)C(C)COO + CC(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)COO + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)COO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[C](C)C(=O)C(C)COO | No |
| C[C](C)C(=O)C(C)COO + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| C[C](C)C(=O)C(C)COO + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)C(=O)C(C)COO + [H] ↔ [H][H] + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + [O] ↔ [OH] + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [OH] ↔ O + C[C](C)C(=O)C(C)COO | No |
| C[C](C)C(=O)C(C)COO + OO ↔ CC(C)C(=O)C(C)COO + [O]O | No |
| CC(C)C(=O)C(C)COO + C#C[CH2] ↔ C#CC + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C=C ↔ C=C=C + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [c]1ccccc1 ↔ c1ccccc1 + C[C](C)C(=O)C(C)COO | No |
| C[C](C)C(=O)C(C)COO + C=CC ↔ CC(C)C(=O)C(C)COO + [CH2]C=C | No |
| C[C](C)C(=O)C(C)COO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)COO + C=C1[CH]CC=C1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C[C](C)C(=O)C(C)COO + C=C1CC=CC1 ↔ CC(C)C(=O)C(C)COO + C=C1[CH]C=CC1 | Yes |
| C[C](C)C(=O)C(C)COO + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)COO + C=C1C=C[CH]C1 | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C ↔ C=C + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH]=CC ↔ C=CC + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + C=[C]C ↔ C=CC + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + [CH3] ↔ C + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + [CH2]CC ↔ CCC + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + C[CH]C ↔ CCC + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH2] ↔ [CH3] + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + C[CH]O ↔ CCO + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + [CH2]CO ↔ CCO + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + CC[O] ↔ CCO + C[C](C)C(=O)C(C)COO | Yes |
| C[C](C)C(=O)C(C)COO + CC=O ↔ CC(C)C(=O)C(C)COO + C[C]=O | Yes |
| CC(C)C(=O)C(C)COO + [CH2]C=O ↔ CC=O + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + C[CH2] ↔ CC + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C=O ↔ C=C=O + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH2]O ↔ CO + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + [C]#C ↔ C#C + C[C](C)C(=O)C(C)COO | No |
| C[C](C)C(=O)C(C)COO + C=O ↔ CC(C)C(=O)C(C)COO + [CH]=O | Yes |
| CC(C)C(=O)C(C)COO + [CH2]C=C=O ↔ CC=C=O + C[C](C)C(=O)C(C)COO | No |
| C[C](C)C(=O)C(C)COO + C=CC=O ↔ CC(C)C(=O)C(C)COO + C=C[C]=O | Yes |
| CC(C)C(=O)C(C)COO + [CH]=CC#C ↔ C#CC=C + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + C#C[C]=C ↔ C#CC=C + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + C[C](C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + C[C](C)C(=O)C(C)COO | No |
| CC(C)C(=O)C(C)COO + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + [CH2]C(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + C[C](C)C(=O)C(C)COO | Yes |
| [CH2]C(C)=C=O + [O]O ↔ CC(C)=C=O + [O][O] | Yes |
| CC(C)=C=O + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C(C)=C=O | No |
| CC(C)=C=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C(C)=C=O | Yes |
| [CH2]C(C)=C=O + CC(C)C(=O)C(C)(C)OO ↔ CC(C)=C=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C(C)=C=O + CC(C)C(=O)C(C)COO ↔ CC(C)=C=O + CC(C)C(=O)C(C)CO[O] | No |
| CC(C)=C=O + [H] ↔ [H][H] + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [O] ↔ [OH] + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [OH] ↔ O + [CH2]C(C)=C=O | No |
| [CH2]C(C)=C=O + OO ↔ CC(C)=C=O + [O]O | No |
| CC(C)=C=O + C#C[CH2] ↔ C#CC + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH]=C=C ↔ C=C=C + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C(C)=C=O | No |
| CC(C)=C=O + [CH2]C=C ↔ C=CC + [CH2]C(C)=C=O | Yes |
| [CH2]C(C)=C=O + C=C1C=CCC1 ↔ CC(C)=C=O + C=C1[CH]CC=C1 | Yes |
| [CH2]C(C)=C=O + C=C1CC=CC1 ↔ CC(C)=C=O + C=C1[CH]C=CC1 | Yes |
| [CH2]C(C)=C=O + C=C1C=CCC1 ↔ CC(C)=C=O + C=C1C=C[CH]C1 | Yes |
| CC(C)=C=O + [CH]=C ↔ C=C + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH]=CC ↔ C=CC + [CH2]C(C)=C=O | No |
| CC(C)=C=O + C=[C]C ↔ C=CC + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH3] ↔ C + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH2]CC ↔ CCC + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + C[CH]C ↔ CCC + [CH2]C(C)=C=O | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC(C)=C=O + [CH2] ↔ [CH3] + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + C[CH]O ↔ CCO + [CH2]C(C)=C=O | No |
| CC(C)=C=O + [CH2]CO ↔ CCO + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + CC[O] ↔ CCO + [CH2]C(C)=C=O | No |
| CC(C)=C=O + C[C]=O ↔ CC=O + [CH2]C(C)=C=O | No |
| CC(C)=C=O + [CH2]C=O ↔ CC=O + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + C[CH2] ↔ CC + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH]=C=O ↔ C=C=O + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH2]O ↔ CO + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [C]#C ↔ C#C + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH]=O ↔ C=O + [CH2]C(C)=C=O | No |
| CC(C)=C=O + [CH2]C=C=O ↔ CC=C=O + [CH2]C(C)=C=O | No |
| CC(C)=C=O + C=C[C]=O ↔ C=CC=O + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH]=CC#C ↔ C#CC=C + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + C#C[C]=C ↔ C#CC=C + [CH2]C(C)=C=O | No |
| CC(C)=C=O + C[C](C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]C(C)=C=O | Yes |
| CC(C)=C=O + [CH2]C(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C(C)=C=O | No |
| CC(C)=C=O + C[C](C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)COO + [CH2]C(C)=C=O | Yes |
| [CH2]C(C)C(=O)C(C)C + C=C(C)C(=O)OO ↔ CC(C)C(=O)C(C)C + C=C(C)C(=O)O[O] | Yes |
| CC(C)C(=O)C(C)C + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[C](C)C(=O)C(C)C | No |
| [CH2]C(C)C(=O)C(C)(C)OO + C=C(C)C(=O)OO ↔ CC(C)C(=O)C(C)(C)OO + C=C(C)C(=O)O[O] | Yes |
| CC(C)C(=O)C(C)(C)OO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[C](C)C(=O)C(C)(C)OO | No |
| CC(C)C(=O)C(C)(C)OO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| CC(C)C(=O)C(C)COO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[C](C)C(=O)C(C)COO | Yes |
| CC(C)C(=O)C(C)COO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + CC(C)C(=O)C(C)CO[O] | Yes |
| [H] + C=C(C)C(=O)OO ↔ [H][H] + C=C(C)C(=O)O[O] | Yes |
| [OH] + C=C(C)C(=O)OO ↔ O + C=C(C)C(=O)O[O] | Yes |
| [O]O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [O][O] | No |
| OO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [O]O | Yes |
| [c]1ccccc1 + C=C(C)C(=O)OO ↔ c1ccccc1 + C=C(C)C(=O)O[O] | No |
| C=C1C=CCC1 + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C=C1[CH]CC=C1 | Yes |
| C=C1CC=CC1 + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C=C1[CH]C=CC1 | Yes |
| C=C=C + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH]=C=C | Yes |
| C#CC + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C#C[CH2] | No |
| [C]#C + C=C(C)C(=O)OO ↔ C#C + C=C(C)C(=O)O[O] | Yes |
| [CH]=CC + C=C(C)C(=O)OO ↔ C=CC + C=C(C)C(=O)O[O] | No |
| C=[C]C + C=C(C)C(=O)OO ↔ C=CC + C=C(C)C(=O)O[O] | No |
| C=CC + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]C=C | No |
| [CH]=C + C=C(C)C(=O)OO ↔ C=C + C=C(C)C(=O)O[O] | Yes |
| [CH]=C=O + C=C(C)C(=O)OO ↔ C=C=O + C=C(C)C(=O)O[O] | No |
| C=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH]=O | No |
| CO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]O | Yes |
| [CH3] + C=C(C)C(=O)OO ↔ C + C=C(C)C(=O)O[O] | Yes |
| [CH2]CO + C=C(C)C(=O)OO ↔ CCO + C=C(C)C(=O)O[O] | No |
| CCO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[CH]O | No |
| CC[O] + C=C(C)C(=O)OO ↔ CCO + C=C(C)C(=O)O[O] | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]C=O | No |
| CC=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[C]=O | Yes |
| C[CH2] + C=C(C)C(=O)OO ↔ CC + C=C(C)C(=O)O[O] | No |
| [CH2]CC + C=C(C)C(=O)OO ↔ CCC + C=C(C)C(=O)O[O] | No |
| CCC + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C[CH]C | No |
| CC=C=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]C=C=O | Yes |
| C=CC=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + C=C[C]=O | No |
| C#C[C]=C + C=C(C)C(=O)OO ↔ C#CC=C + C=C(C)C(=O)O[O] | No |
| [CH]=CC#C + C=C(C)C(=O)OO ↔ C#CC=C + C=C(C)C(=O)O[O] | No |
| CC(C)=C=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]C(C)=C=O | No |
| CC(C)C(=O)OO + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + CC(C)C(=O)O[O] | No |
| C=C(C)C(=O)OO + [CH2] ↔ [CH3] + C=C(C)C(=O)O[O] | Yes |
| [CH2]C(COO)C(=O)C(C)C + [O]O ↔ CC(C)C(=O)C(C)COO + [O][O] | No |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)COO + C[C](C)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)COO + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)C(=O)C(C)COO + [H] ↔ [H][H] + [CH2]C(COO)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)COO + [O] ↔ [OH] + [CH2]C(COO)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)COO + [OH] ↔ O + [CH2]C(COO)C(=O)C(C)C | No |
| [CH2]C(COO)C(=O)C(C)C + OO ↔ CC(C)C(=O)C(C)COO + [O]O | No |
| [CH2]C(COO)C(=O)C(C)C + C#CC ↔ CC(C)C(=O)C(C)COO + C#C[CH2] | Yes |
| [CH2]C(COO)C(=O)C(C)C + C=C=C ↔ CC(C)C(=O)C(C)COO + [CH]=C=C | Yes |
| CC(C)C(=O)C(C)COO + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + C=CC ↔ CC(C)C(=O)C(C)COO + [CH2]C=C | No |
| [CH2]C(COO)C(=O)C(C)C + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)COO + C=C1[CH]CC=C1 | Yes |
| [CH2]C(COO)C(=O)C(C)C + C=C1CC=CC1 ↔ CC(C)C(=O)C(C)COO + C=C1[CH]C=CC1 | No |
| [CH2]C(COO)C(=O)C(C)C + C=C1C=CCC1 ↔ CC(C)C(=O)C(C)COO + C=C1C=C[CH]C1 | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C ↔ C=C + [CH2]C(COO)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)COO + [CH]=CC ↔ C=CC + [CH2]C(COO)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)COO + C=[C]C ↔ C=CC + [CH2]C(COO)C(=O)C(C)C | No |
| CC(C)C(=O)C(C)COO + [CH3] ↔ C + [CH2]C(COO)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)COO + [CH2]CC ↔ CCC + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CCC ↔ CC(C)C(=O)C(C)COO + C[CH]C | Yes |
| CC(C)C(=O)C(C)COO + [CH2] ↔ [CH3] + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CCO ↔ CC(C)C(=O)C(C)COO + C[CH]O | No |
| CC(C)C(=O)C(C)COO + [CH2]CO ↔ CCO + [CH2]C(COO)C(=O)C(C)C | Yes |
| CC(C)C(=O)C(C)COO + CC[O] ↔ CCO + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC=O ↔ CC(C)C(=O)C(C)COO + C[C]=O | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC=O ↔ CC(C)C(=O)C(C)COO + [CH2]C=O | No |
| [CH2]C(COO)C(=O)C(C)C + CC ↔ CC(C)C(=O)C(C)COO + C[CH2] | Yes |
| CC(C)C(=O)C(C)COO + [CH]=C=O ↔ C=C=O + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CO ↔ CC(C)C(=O)C(C)COO + [CH2]O | No |
| CC(C)C(=O)C(C)COO + [C]#C ↔ C#C + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + C=O ↔ CC(C)C(=O)C(C)COO + [CH]=O | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC=C=O ↔ CC(C)C(=O)C(C)COO + [CH2]C=C=O | No |
| [CH2]C(COO)C(=O)C(C)C + C=CC=O ↔ CC(C)C(=O)C(C)COO + C=C[C]=O | Yes |
| CC(C)C(=O)C(C)COO + [CH]=CC#C ↔ C#CC=C + [CH2]C(COO)C(=O)C(C)C | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC(C)C(=O)C(C)COO + C#C[C]=C ↔ C#CC=C + [CH2]C(COO)C(=O)C(C)C | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)COO + C[C](C)C(=O)C(C)(C)OO | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)OO ↔ CC(C)C(=O)C(C)COO + CC(C)C(=O)O[O] | Yes |
| CC(C)C(=O)C(C)COO + [CH2]C(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C(COO)C(=O)C(C)C | No |
| [CH2]C(COO)C(=O)C(C)C + CC(C)C(=O)C(C)COO ↔ CC(C)C(=O)C(C)COO + C[C](C)C(=O)C(C)COO | Yes |
| [CH2]C(COO)C(=O)C(C)C + CC(C)=C=O ↔ CC(C)C(=O)C(C)COO + [CH2]C(C)=C=O | Yes |
| [CH2]C(COO)C(=O)C(C)C + C=C(C)C(=O)OO ↔ CC(C)C(=O)C(C)COO + C=C(C)C(=O)O[O] | No |
| [CH2]C(C)=O + [O]O ↔ CC(C)=O + [O][O] | Yes |
| [CH2]C(C)=O + CC(C)C(=O)C(C)C ↔ CC(C)=O + C[C](C)C(=O)C(C)C | Yes |
| CC(C)=O + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + CC(C)C(=O)C(C)(C)OO ↔ CC(C)=O + CC(C)C(=O)C(C)(C)O[O] | Yes |
| [CH2]C(C)=O + CC(C)C(=O)C(C)COO ↔ CC(C)=O + CC(C)C(=O)C(C)CO[O] | Yes |
| CC(C)=O + [H] ↔ [H][H] + [CH2]C(C)=O | Yes |
| CC(C)=O + [O] ↔ [OH] + [CH2]C(C)=O | Yes |
| CC(C)=O + [OH] ↔ O + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + OO ↔ CC(C)=O + [O]O | No |
| [CH2]C(C)=O + C#CC ↔ CC(C)=O + C#C[CH2] | Yes |
| [CH2]C(C)=O + C=C=C ↔ CC(C)=O + [CH]=C=C | Yes |
| CC(C)=O + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + C=CC ↔ CC(C)=O + [CH2]C=C | Yes |
| [CH2]C(C)=O + C=C1C=CCC1 ↔ CC(C)=O + C=C1[CH]CC=C1 | Yes |
| [CH2]C(C)=O + C=C1CC=CC1 ↔ CC(C)=O + C=C1[CH]C=CC1 | Yes |
| [CH2]C(C)=O + C=C1C=CCC1 ↔ CC(C)=O + C=C1C=C[CH]C1 | Yes |
| CC(C)=O + [CH]=C ↔ C=C + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH]=CC ↔ C=CC + [CH2]C(C)=O | Yes |
| CC(C)=O + C=[C]C ↔ C=CC + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH3] ↔ C + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH2]CC ↔ CCC + [CH2]C(C)=O | Yes |
| CC(C)=O + C[CH]C ↔ CCC + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH2] ↔ [CH3] + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + CCO ↔ CC(C)=O + C[CH]O | No |
| CC(C)=O + [CH2]CO ↔ CCO + [CH2]C(C)=O | Yes |
| CC(C)=O + CC[O] ↔ CCO + [CH2]C(C)=O | No |
| [CH2]C(C)=O + CC=O ↔ CC(C)=O + C[C]=O | Yes |
| [CH2]C(C)=O + CC=O ↔ CC(C)=O + [CH2]C=O | Yes |
| CC(C)=O + C[CH2] ↔ CC + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH]=C=O ↔ C=C=O + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + CO ↔ CC(C)=O + [CH2]O | No |
| CC(C)=O + [C]#C ↔ C#C + [CH2]C(C)=O | Yes |
| [CH2]C(C)=O + C=O ↔ CC(C)=O + [CH]=O | No |
| [CH2]C(C)=O + CC=C=O ↔ CC(C)=O + [CH2]C=C=O | No |
| [CH2]C(C)=O + C=CC=O ↔ CC(C)=O + C=C[C]=O | Yes |
| CC(C)=O + [CH]=CC#C ↔ C#CC=C + [CH2]C(C)=O | Yes |
| CC(C)=O + C#C[C]=C ↔ C#CC=C + [CH2]C(C)=O | No |
| [CH2]C(C)=O + CC(C)C(=O)C(C)(C)OO ↔ CC(C)=O + C[C](C)C(=O)C(C)(C)OO | Yes |
| CC(C)=O + CC(C)C(=O)O[O] ↔ CC(C)C(=O)OO + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH2]C(C)C(=O)C(C)(C)OO ↔ CC(C)C(=O)C(C)(C)OO + [CH2]C(C)=O | No |
| [CH2]C(C)=O + CC(C)C(=O)C(C)COO ↔ CC(C)=O + C[C](C)C(=O)C(C)COO | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| [CH2]C(C)=O + CC(C)=C=O ↔ CC(C)=O + [CH2]C(C)=C=O | No |
| CC(C)=O + C=C(C)C(=O)O[O] ↔ C=C(C)C(=O)OO + [CH2]C(C)=O | Yes |
| CC(C)=O + [CH2]C(COO)C(=O)C(C)C ↔ CC(C)C(=O)C(C)COO + [CH2]C(C)=O | No |
| [CH]=CC=C + C ↔ C=CC=C + [CH3] | Yes |
| C=CC=C + [CH3] ↔ C + C=[C]C=C | No |
| [CH]=CC=C + C=CC ↔ C=CC=C + [CH2]C=C | Yes |
| C=[C]C=C + C=CC ↔ C=CC=C + [CH2]C=C | No |
| C=CC=CC + [CH3] ↔ C + [CH2]C=CC=C | Yes |
| C=CC=CC + [CH2]C=C ↔ C=CC + [CH2]C=CC=C | No |
| C1=CCCC=C1 + [CH3] ↔ C + [CH]1C=CC=CC1 | Yes |
| C1=CCCC=C1 + [CH2]C=C ↔ C=CC + [CH]1C=CC=CC1 | Yes |
| [CH]=CC=C + CC(C)C(=O)C(C)C ↔ C=CC=C + C[C](C)C(=O)C(C)C | Yes |
| C=[C]C=C + CC(C)C(=O)C(C)C ↔ C=CC=C + C[C](C)C(=O)C(C)C | Yes |
| C=CC=CC + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C=CC=C | No |
| C1=CCCC=C1 + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]1C=CC=CC1 | Yes |
| [CH]=CC=C + CC(C)C(=O)C(C)C ↔ C=CC=C + [CH2]C(C)C(=O)C(C)C | Yes |
| C=[C]C=C + CC(C)C(=O)C(C)C ↔ C=CC=C + [CH2]C(C)C(=O)C(C)C | Yes |
| C=CC=CC + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]1C=CC=CC1 | Yes |
| [H] + C=CC=CC ↔ [H][H] + [CH2]C=CC=C | Yes |
| [C]#C + C=CC=CC ↔ C#C + [CH2]C=CC=C | No |
| [CH]=C + C=CC=CC ↔ C=C + [CH2]C=CC=C | Yes |
| [CH]=CC + C=CC=CC ↔ C=CC + [CH2]C=CC=C | No |
| C=[C]C + C=CC=CC ↔ C=CC + [CH2]C=CC=C | Yes |
| [CH]=C=C + C=CC=CC ↔ C=C=C + [CH2]C=CC=C | Yes |
| C#C[CH2] + C=CC=CC ↔ C#CC + [CH2]C=CC=C | Yes |
| [CH]=CC#C + C=CC=CC ↔ C#CC=C + [CH2]C=CC=C | Yes |
| C#C[C]=C + C=CC=CC ↔ C#CC=C + [CH2]C=CC=C | No |
| [CH]=CC=C + C=CC=CC ↔ C=CC=C + [CH2]C=CC=C | Yes |
| C=[C]C=C + C=CC=CC ↔ C=CC=C + [CH2]C=CC=C | Yes |
| [CH2]C=C=O + C=CC=CC ↔ CC=C=O + [CH2]C=CC=C | No |
| [c]1ccccc1 + C=CC=CC ↔ c1ccccc1 + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + [CH2]C=CC=C ↔ C=CC=CC + [CH]1C=CC=CC1 | No |
| [H] + C1=CCCC=C1 ↔ [H][H] + [CH]1C=CC=CC1 | Yes |
| [C]#C + C1=CCCC=C1 ↔ C#C + [CH]1C=CC=CC1 | Yes |
| [CH]=C + C1=CCCC=C1 ↔ C=C + [CH]1C=CC=CC1 | No |
| [CH]=CC + C1=CCCC=C1 ↔ C=CC + [CH]1C=CC=CC1 | Yes |
| C=[C]C + C1=CCCC=C1 ↔ C=CC + [CH]1C=CC=CC1 | Yes |
| [CH]=C=C + C1=CCCC=C1 ↔ C=C=C + [CH]1C=CC=CC1 | No |
| C#C[CH2] + C1=CCCC=C1 ↔ C#CC + [CH]1C=CC=CC1 | No |
| [CH]=CC#C + C1=CCCC=C1 ↔ C#CC=C + [CH]1C=CC=CC1 | No |
| C#C[C]=C + C1=CCCC=C1 ↔ C#CC=C + [CH]1C=CC=CC1 | Yes |
| [CH]=CC=C + C1=CCCC=C1 ↔ C=CC=C + [CH]1C=CC=CC1 | No |
| C=[C]C=C + C1=CCCC=C1 ↔ C=CC=C + [CH]1C=CC=CC1 | Yes |
| [CH2]C=C=O + C1=CCCC=C1 ↔ CC=C=O + [CH]1C=CC=CC1 | No |
| [c]1ccccc1 + C1=CCCC=C1 ↔ c1ccccc1 + [CH]1C=CC=CC1 | Yes |
| [CH]=CC=C + [H][H] ↔ C=CC=C + [H] | No |
| C=CC=C + [H] ↔ [H][H] + C=[C]C=C | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=CC=C + [O] ↔ [OH] + C=[C]C=C | Yes |
| C=CC=CC + [O] ↔ [OH] + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + [O] ↔ [OH] + [CH]1C=CC=CC1 | No |
| C=CC=C + [OH] ↔ O + [CH]=CC=C | No |
| C=CC=C + [OH] ↔ O + C=[C]C=C | Yes |
| C=CC=CC + [OH] ↔ O + [CH2]C=CC=C | No |
| C1=CCCC=C1 + [OH] ↔ O + [CH]1C=CC=CC1 | No |
| [CH]=CC=C + [O]O ↔ C=CC=C + [O][O] | No |
| C=[C]C=C + [O]O ↔ C=CC=C + [O][O] | No |
| [CH2]C=CC=C + [O]O ↔ C=CC=CC + [O][O] | Yes |
| [CH]1C=CC=CC1 + [O]O ↔ C1=CCCC=C1 + [O][O] | Yes |
| [CH]=CC=C + OO ↔ C=CC=C + [O]O | Yes |
| C=[C]C=C + OO ↔ C=CC=C + [O]O | No |
| C=CC=CC + [O]O ↔ OO + [CH2]C=CC=C | No |
| C1=CCCC=C1 + [O]O ↔ OO + [CH]1C=CC=CC1 | No |
| [CH]=CC=C + C#CC ↔ C=CC=C + C#C[CH2] | No |
| C=[C]C=C + C#CC ↔ C=CC=C + C#C[CH2] | Yes |
| [CH]=CC=C + C=C=C ↔ C=CC=C + [CH]=C=C | No |
| C=[C]C=C + C=C=C ↔ C=CC=C + [CH]=C=C | Yes |
| C=CC=C + [c]1ccccc1 ↔ c1ccccc1 + [CH]=CC=C | No |
| C=CC=C + [c]1ccccc1 ↔ c1ccccc1 + C=[C]C=C | Yes |
| C=C1C=CCC1 + [CH2]C=CC=C ↔ C=CC=CC + C=C1C=C[CH]C1 | Yes |
| C=C1[CH]CC=C1 + C=CC=CC ↔ C=C1C=CCC1 + [CH2]C=CC=C | Yes |
| C=C1C=C[CH]C1 + C1=CCCC=C1 ↔ C=C1C=CCC1 + [CH]1C=CC=CC1 | Yes |
| C=C1[CH]CC=C1 + C1=CCCC=C1 ↔ C=C1C=CCC1 + [CH]1C=CC=CC1 | Yes |
| C=C1CC=CC1 + [CH2]C=CC=C ↔ C=CC=CC + C=C1[CH]C=CC1 | Yes |
| C=C1CC=CC1 + [CH]1C=CC=CC1 ↔ C1=CCCC=C1 + C=C1[CH]C=CC1 | Yes |
| [C]#C + C=CC=C ↔ C#C + C=[C]C=C | Yes |
| [CH]=C + C=CC=C ↔ C=C + C=[C]C=C | No |
| [CH]=CC + C=CC=C ↔ C=CC + C=[C]C=C | No |
| C=[C]C + C=CC=C ↔ C=CC + C=[C]C=C | Yes |
| [CH]=CC#C + C=CC=C ↔ C#CC=C + C=[C]C=C | Yes |
| C#CC=C + C=[C]C=C ↔ C=CC=C + C#C[C]=C | Yes |
| [CH]=CC=C + C=CC=C ↔ C=CC=C + C=[C]C=C | No |
| CC=C=O + C=[C]C=C ↔ C=CC=C + [CH2]C=C=O | No |
| C=C1C=CCC1 + C=[C]C=C ↔ C=CC=C + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + C=[C]C=C ↔ C=CC=C + C=C1[CH]CC=C1 | No |
| C=C1CC=CC1 + C=[C]C=C ↔ C=CC=C + C=C1[CH]C=CC1 | No |
| [CH]=CC=C + C=C1C=CCC1 ↔ C=CC=C + C=C1[CH]CC=C1 | No |
| [CH]=CC=C + C=C1CC=CC1 ↔ C=CC=C + C=C1[CH]C=CC1 | Yes |
| [CH]=CC=C + C=C1C=CCC1 ↔ C=CC=C + C=C1C=C[CH]C1 | No |
| [CH]=CC=C + C=C ↔ C=CC=C + [CH]=C | No |
| [CH]=CC=C + C=CC ↔ C=CC=C + [CH]=CC | Yes |
| [CH]=CC=C + C=CC ↔ C=CC=C + C=[C]C | Yes |
| [CH]=CC=C + CCC ↔ C=CC=C + [CH2]CC | Yes |
| C=[C]C=C + CCC ↔ C=CC=C + [CH2]CC | Yes |
| C=CC=CC + [CH2]CC ↔ CCC + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + [CH2]CC ↔ CCC + [CH]1C=CC=CC1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| [CH]=CC=C + CCC ↔ C=CC=C + C[CH]C | Yes |
| C=[C]C=C + CCC ↔ C=CC=C + C[CH]C | Yes |
| C=CC=CC + C[CH]C ↔ CCC + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + C[CH]C ↔ CCC + [CH]1C=CC=CC1 | Yes |
| [CH]=C=O + C=CC=CC ↔ C=C=O + [CH2]C=CC=C | Yes |
| [CH]=C=O + C1=CCCC=C1 ↔ C=C=O + [CH]1C=CC=CC1 | Yes |
| [CH]=C=O + C=CC=C ↔ C=C=O + C=[C]C=C | Yes |
| [CH]=O + C=CC=CC ↔ C=O + [CH2]C=CC=C | Yes |
| [CH]=O + C1=CCCC=C1 ↔ C=O + [CH]1C=CC=CC1 | Yes |
| C=O + C=[C]C=C ↔ C=CC=C + [CH]=O | Yes |
| [CH2]O + C=CC=CC ↔ CO + [CH2]C=CC=C | No |
| [CH2]O + C1=CCCC=C1 ↔ CO + [CH]1C=CC=CC1 | Yes |
| CO + C=[C]C=C ↔ C=CC=C + [CH2]O | Yes |
| C=CC=C + [CH2] ↔ [CH3] + C=[C]C=C | No |
| C=CC=CC + [CH2] ↔ [CH3] + [CH2]C=CC=C | Yes |
| C1=CCCC=C1 + [CH2] ↔ [CH3] + [CH]1C=CC=CC1 | Yes |
| [CH2]CO + C=CC=CC ↔ CCO + [CH2]C=CC=C | No |
| C[CH]O + C=CC=CC ↔ CCO + [CH2]C=CC=C | Yes |
| CC[O] + C=CC=CC ↔ CCO + [CH2]C=CC=C | Yes |
| [CH2]CO + C1=CCCC=C1 ↔ CCO + [CH]1C=CC=CC1 | No |
| C[CH]O + C1=CCCC=C1 ↔ CCO + [CH]1C=CC=CC1 | No |
| CC[O] + C1=CCCC=C1 ↔ CCO + [CH]1C=CC=CC1 | Yes |
| [CH2]CO + C=CC=C ↔ CCO + C=[C]C=C | No |
| CCO + C=[C]C=C ↔ C=CC=C + C[CH]O | Yes |
| CC[O] + C=CC=C ↔ CCO + C=[C]C=C | Yes |
| [CH]=CC=C + CCO ↔ C=CC=C + C[CH]O | Yes |
| [CH]=CC=C + CCO ↔ C=CC=C + [CH2]CO | No |
| [CH]=CC=C + CCO ↔ C=CC=C + CC[O] | Yes |
| [CH2]C=O + C=CC=CC ↔ CC=O + [CH2]C=CC=C | No |
| C[C]=O + C=CC=CC ↔ CC=O + [CH2]C=CC=C | Yes |
| [CH2]C=O + C1=CCCC=C1 ↔ CC=O + [CH]1C=CC=CC1 | Yes |
| C[C]=O + C1=CCCC=C1 ↔ CC=O + [CH]1C=CC=CC1 | Yes |
| CC=O + C=[C]C=C ↔ C=CC=C + [CH2]C=O | Yes |
| CC=O + C=[C]C=C ↔ C=CC=C + C[C]=O | No |
| [CH]=CC=C + CC=O ↔ C=CC=C + C[C]=O | No |
| [CH]=CC=C + CC=O ↔ C=CC=C + [CH2]C=O | Yes |
| [CH]=CC=C + CC ↔ C=CC=C + C[CH2] | Yes |
| C=[C]C=C + CC ↔ C=CC=C + C[CH2] | Yes |
| C=CC=CC + C[CH2] ↔ CC + [CH2]C=CC=C | No |
| C1=CCCC=C1 + C[CH2] ↔ CC + [CH]1C=CC=CC1 | Yes |
| [CH]=CC=C + C=C=O ↔ C=CC=C + [CH]=C=O | Yes |
| [CH]=CC=C + CO ↔ C=CC=C + [CH2]O | No |
| C=CC=C + [C]#C ↔ C#C + [CH]=CC=C | Yes |
| [CH]=CC=C + C=O ↔ C=CC=C + [CH]=O | Yes |
| [CH]=CC=C + CC=C=O ↔ C=CC=C + [CH2]C=C=O | No |
| [CH]=CC=C + C=CC=O ↔ C=CC=C + C=C[C]=O | No |
| C=[C]C=C + C=CC=O ↔ C=CC=C + C=C[C]=O | Yes |
| C=CC=CC + C=C[C]=O ↔ C=CC=O + [CH2]C=CC=C | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C1=CCCC=C1 + C=C[C]=O ↔ C=CC=O + [CH]1C=CC=CC1 | Yes |
| C=CC=C + [CH]=CC#C ↔ C#CC=C + [CH]=CC=C | Yes |
| [CH]=CC=C + C#CC=C ↔ C=CC=C + C#C[C]=C | Yes |
| CCC(=O)C(C)C + [CH3] ↔ C + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + C=CC ↔ CCC(=O)C(C)C + [CH2]C=C | Yes |
| C[CH]C(=O)C(C)C + CC(C)C(=O)C(C)C ↔ CCC(=O)C(C)C + C[C](C)C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + C=CC=CC ↔ CCC(=O)C(C)C + [CH2]C=CC=C | Yes |
| C[CH]C(=O)C(C)C + C1=CCCC=C1 ↔ CCC(=O)C(C)C + [CH]1C=CC=CC1 | Yes |
| CCC(=O)C(C)C + [H] ↔ [H][H] + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [O] ↔ [OH] + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [OH] ↔ O + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + [O]O ↔ CCC(=O)C(C)C + [O][O] | No |
| C[CH]C(=O)C(C)C + OO ↔ CCC(=O)C(C)C + [O]O | No |
| C[CH]C(=O)C(C)C + C#CC ↔ CCC(=O)C(C)C + C#C[CH2] | Yes |
| C[CH]C(=O)C(C)C + C=C=C ↔ CCC(=O)C(C)C + [CH]=C=C | Yes |
| CCC(=O)C(C)C + [c]1ccccc1 ↔ c1ccccc1 + C[CH]C(=O)C(C)C | No |
| CCC(=O)C(C)C + C=[C]C=C ↔ C=CC=C + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + C=C1C=CCC1 ↔ CCC(=O)C(C)C + C=C1[CH]CC=C1 | Yes |
| C[CH]C(=O)C(C)C + C=C1CC=CC1 ↔ CCC(=O)C(C)C + C=C1[CH]C=CC1 | Yes |
| C[CH]C(=O)C(C)C + C=C1C=CCC1 ↔ CCC(=O)C(C)C + C=C1C=C[CH]C1 | Yes |
| CCC(=O)C(C)C + [CH]=C ↔ C=C + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [CH]=CC ↔ C=CC + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + C=[C]C ↔ C=CC + C[CH]C(=O)C(C)C | No |
| CCC(=O)C(C)C + [CH2]CC ↔ CCC + C[CH]C(=O)C(C)C | No |
| CCC(=O)C(C)C + C[CH]C ↔ CCC + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [CH2] ↔ [CH3] + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + CCO ↔ CCC(=O)C(C)C + C[CH]O | No |
| CCC(=O)C(C)C + [CH2]CO ↔ CCO + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + CC[O] ↔ CCO + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + CC=O ↔ CCC(=O)C(C)C + C[C]=O | No |
| C[CH]C(=O)C(C)C + CC=O ↔ CCC(=O)C(C)C + [CH2]C=O | Yes |
| CCC(=O)C(C)C + C[CH2] ↔ CC + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [CH]=C=O ↔ C=C=O + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + CO ↔ CCC(=O)C(C)C + [CH2]O | Yes |
| CCC(=O)C(C)C + [C]#C ↔ C#C + C[CH]C(=O)C(C)C | Yes |
| C[CH]C(=O)C(C)C + C=O ↔ CCC(=O)C(C)C + [CH]=O | Yes |
| C[CH]C(=O)C(C)C + CC=C=O ↔ CCC(=O)C(C)C + [CH2]C=C=O | No |
| C[CH]C(=O)C(C)C + C=CC=O ↔ CCC(=O)C(C)C + C=C[C]=O | Yes |
| CCC(=O)C(C)C + [CH]=CC#C ↔ C#CC=C + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + C#C[C]=C ↔ C#CC=C + C[CH]C(=O)C(C)C | Yes |
| CCC(=O)C(C)C + [CH]=CC=C ↔ C=CC=C + C[CH]C(=O)C(C)C | Yes |
| C=CCC + [CH3] ↔ C + C=C[CH]C | No |
| C=CCC + [CH2]C=C ↔ C=CC + C=C[CH]C | Yes |
| C=CCC + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C[CH]C | Yes |
| C=CCC + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + C=C[CH]C | Yes |
| C=C[CH]C + C=CC=CC ↔ C=CCC + [CH2]C=CC=C | Yes |
| C=C[CH]C + C1=CCCC=C1 ↔ C=CCC + [CH]1C=CC=CC1 | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=CCC + [H] ↔ [H][H] + C=C[CH]C | Yes |
| C=CCC + [O] ↔ [OH] + C=C[CH]C | No |
| C=CCC + [OH] ↔ O + C=C[CH]C | No |
| C=C[CH]C + [O]O ↔ C=CCC + [O][O] | No |
| C=CCC + [O]O ↔ OO + C=C[CH]C | Yes |
| C=CCC + C#C[CH2] ↔ C#CC + C=C[CH]C | No |
| C=CCC + [CH]=C=C ↔ C=C=C + C=C[CH]C | Yes |
| C=CCC + [c]1ccccc1 ↔ c1ccccc1 + C=C[CH]C | No |
| C=CCC + C=[C]C=C ↔ C=CC=C + C=C[CH]C | Yes |
| C=CCC + C=C1[CH]CC=C1 ↔ C=C1C=CCC1 + C=C[CH]C | No |
| C=C[CH]C + C=C1CC=CC1 ↔ C=CCC + C=C1[CH]C=CC1 | Yes |
| C=C[CH]C + C=C1C=CCC1 ↔ C=CCC + C=C1C=C[CH]C1 | Yes |
| C=CCC + [CH]=C ↔ C=C + C=C[CH]C | Yes |
| C=CCC + [CH]=CC ↔ C=CC + C=C[CH]C | Yes |
| C=CCC + C=[C]C ↔ C=CC + C=C[CH]C | Yes |
| C=CCC + [CH2]CC ↔ CCC + C=C[CH]C | Yes |
| C=CCC + C[CH]C ↔ CCC + C=C[CH]C | No |
| C=CCC + [CH2] ↔ [CH3] + C=C[CH]C | Yes |
| C=CCC + C[CH]O ↔ CCO + C=C[CH]C | No |
| C=CCC + [CH2]CO ↔ CCO + C=C[CH]C | Yes |
| C=CCC + CC[O] ↔ CCO + C=C[CH]C | Yes |
| C=CCC + C[C]=O ↔ CC=O + C=C[CH]C | No |
| C=CCC + [CH2]C=O ↔ CC=O + C=C[CH]C | Yes |
| C=CCC + C[CH2] ↔ CC + C=C[CH]C | Yes |
| C=CCC + [CH]=C=O ↔ C=C=O + C=C[CH]C | Yes |
| C=CCC + [CH2]O ↔ CO + C=C[CH]C | Yes |
| C=CCC + [C]#C ↔ C#C + C=C[CH]C | Yes |
| C=CCC + [CH]=O ↔ C=O + C=C[CH]C | No |
| C=CCC + [CH2]C=C=O ↔ CC=C=O + C=C[CH]C | No |
| C=CCC + C=C[C]=O ↔ C=CC=O + C=C[CH]C | No |
| C=CCC + [CH]=CC#C ↔ C#CC=C + C=C[CH]C | Yes |
| C=CCC + C#C[C]=C ↔ C#CC=C + C=C[CH]C | Yes |
| C=CCC + [CH]=CC=C ↔ C=CC=C + C=C[CH]C | No |
| C=CCC + C[CH]C(=O)C(C)C ↔ CCC(=O)C(C)C + C=C[CH]C | Yes |
| C1=CCC=C1 + [CH3] ↔ C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH2]C=C ↔ C=CC + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C[C](C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH2]C(C)C(=O)C(C)C ↔ CC(C)C(=O)C(C)C + [CH]1C=CC=C1 | Yes |
| [CH]1C=CC=C1 + C=CC=CC ↔ C1=CCC=C1 + [CH2]C=CC=C | No |
| [CH]1C=CC=C1 + C1=CCCC=C1 ↔ C1=CCC=C1 + [CH]1C=CC=CC1 | Yes |
| C1=CCC=C1 + [H] ↔ [H][H] + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [O] ↔ [OH] + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [OH] ↔ O + [CH]1C=CC=C1 | No |
| [CH]1C=CC=C1 + [O]O ↔ C1=CCC=C1 + [O][O] | No |
| C1=CCC=C1 + [O]O ↔ OO + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C#C[CH2] ↔ C#CC + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + [CH]=C=C ↔ C=C=C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [c]1ccccc1 ↔ c1ccccc1 + [CH]1C=CC=C1 | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C1=CCC=C1 + C=[C]C=C ↔ C=CC=C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C=C1[CH]CC=C1 ↔ C=C1C=CCC1 + [CH]1C=CC=C1 | No |
| [CH]1C=CC=C1 + C=C1CC=CC1 ↔ C1=CCC=C1 + C=C1[CH]C=CC1 | Yes |
| [CH]1C=CC=C1 + C=C1C=CCC1 ↔ C1=CCC=C1 + C=C1C=C[CH]C1 | Yes |
| C1=CCC=C1 + [CH]=C ↔ C=C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH]=CC ↔ C=CC + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + C=[C]C ↔ C=CC + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH2]CC ↔ CCC + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + C[CH]C ↔ CCC + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH2] ↔ [CH3] + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C[CH]O ↔ CCO + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + [CH2]CO ↔ CCO + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + CC[O] ↔ CCO + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + C[C]=O ↔ CC=O + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + [CH2]C=O ↔ CC=O + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C[CH2] ↔ CC + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH]=C=O ↔ C=C=O + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH2]O ↔ CO + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [C]#C ↔ C#C + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + [CH]=O ↔ C=O + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + [CH2]C=C=O ↔ CC=C=O + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + C=C[C]=O ↔ C=CC=O + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH]=CC#C ↔ C#CC=C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C#C[C]=C ↔ C#CC=C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH]=CC=C ↔ C=CC=C + [CH]1C=CC=C1 | No |
| C1=CCC=C1 + C[CH]C(=O)C(C)C ↔ CCC(=O)C(C)C + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + C=C[CH]C ↔ C=CCC + [CH]1C=CC=C1 | Yes |
| C1=CCC=C1 + [CH3] ↔ C + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + C=CC ↔ C1=CCC=C1 + [CH2]C=C | Yes |
| [C]1=CCC=C1 + CC(C)C(=O)C(C)C ↔ C1=CCC=C1 + C[C](C)C(=O)C(C)C | Yes |
| [C]1=CCC=C1 + CC(C)C(=O)C(C)C ↔ C1=CCC=C1 + [CH2]C(C)C(=O)C(C)C | Yes |
| [C]1=CCC=C1 + C=CC=CC ↔ C1=CCC=C1 + [CH2]C=CC=C | Yes |
| [C]1=CCC=C1 + C1=CCCC=C1 ↔ C1=CCC=C1 + [CH]1C=CC=CC1 | Yes |
| C1=CCC=C1 + [H] ↔ [H][H] + [C]1=CCC=C1 | Yes |
| C1=CCC=C1 + [O] ↔ [OH] + [C]1=CCC=C1 | Yes |
| C1=CCC=C1 + [OH] ↔ O + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + [O]O ↔ C1=CCC=C1 + [O][O] | No |
| [C]1=CCC=C1 + OO ↔ C1=CCC=C1 + [O]O | No |
| [C]1=CCC=C1 + C#CC ↔ C1=CCC=C1 + C#C[CH2] | Yes |
| [C]1=CCC=C1 + C=C=C ↔ C1=CCC=C1 + [CH]=C=C | Yes |
| C1=CCC=C1 + [c]1ccccc1 ↔ c1ccccc1 + [C]1=CCC=C1 | No |
| [C]1=CCC=C1 + C=CC=C ↔ C1=CCC=C1 + C=[C]C=C | Yes |
| [C]1=CCC=C1 + C=C1C=CCC1 ↔ C1=CCC=C1 + C=C1[CH]CC=C1 | Yes |
| [C]1=CCC=C1 + C=C1CC=CC1 ↔ C1=CCC=C1 + C=C1[CH]C=CC1 | Yes |
| [C]1=CCC=C1 + C=C1C=CCC1 ↔ C1=CCC=C1 + C=C1C=C[CH]C1 | Yes |
| C1=CCC=C1 + [CH]=C ↔ C=C + [C]1=CCC=C1 | Yes |
| C1=CCC=C1 + [CH]=CC ↔ C=CC + [C]1=CCC=C1 | Yes |
| C1=CCC=C1 + C=[C]C ↔ C=CC + [C]1=CCC=C1 | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| [C]1=CCC=C1 + CCC ↔ C1=CCC=C1 + [CH2]CC | No |
| [C]1=CCC=C1 + CCC ↔ C1=CCC=C1 + C[CH]C | Yes |
| C1=CCC=C1 + [CH2] ↔ [CH3] + [C]1=CCC=C1 | No |
| [C]1=CCC=C1 + CCO ↔ C1=CCC=C1 + C[CH]O | No |
| C1=CCC=C1 + [CH2]CO ↔ CCO + [C]1=CCC=C1 | Yes |
| C1=CCC=C1 + CC[O] ↔ CCO + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + CC=O ↔ C1=CCC=C1 + C[C]=O | Yes |
| [C]1=CCC=C1 + CC=O ↔ C1=CCC=C1 + [CH2]C=O | Yes |
| [C]1=CCC=C1 + CC ↔ C1=CCC=C1 + C[CH2] | Yes |
| C1=CCC=C1 + [CH]=C=O ↔ C=C=O + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + CO ↔ C1=CCC=C1 + [CH2]O | Yes |
| C1=CCC=C1 + [C]#C ↔ C#C + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + C=O ↔ C1=CCC=C1 + [CH]=O | Yes |
| [C]1=CCC=C1 + CC=C=O ↔ C1=CCC=C1 + [CH2]C=C=O | No |
| [C]1=CCC=C1 + C=CC=O ↔ C1=CCC=C1 + C=C[C]=O | Yes |
| C1=CCC=C1 + [CH]=CC#C ↔ C#CC=C + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + C#CC=C ↔ C1=CCC=C1 + C#C[C]=C | Yes |
| C1=CCC=C1 + [CH]=CC=C ↔ C=CC=C + [C]1=CCC=C1 | Yes |
| [C]1=CCC=C1 + CCC(=O)C(C)C ↔ C1=CCC=C1 + C[CH]C(=O)C(C)C | Yes |
| [C]1=CCC=C1 + C=CCC ↔ C1=CCC=C1 + C=C[CH]C | Yes |
| [C]1=CCC=C1 + C1=CCC=C1 ↔ C1=CCC=C1 + [CH]1C=CC=C1 | Yes |
| [CH2]C(C)C(=O)C(C)C + C=C=C=C ↔ CC(C)C(=O)C(C)C + [CH]=C=C=C | Yes |
| CC(C)C(=O)C(C)C + [CH]=C=C=C ↔ C=C=C=C + C[C](C)C(=O)C(C)C | Yes |
| [H] + C=C=C=C ↔ [H][H] + [CH]=C=C=C | No |
| [CH3] + C=C=C=C ↔ C + [CH]=C=C=C | Yes |
| [C]#C + C=C=C=C ↔ C#C + [CH]=C=C=C | Yes |
| [CH]=C + C=C=C=C ↔ C=C + [CH]=C=C=C | No |
| [CH]=CC + C=C=C=C ↔ C=CC + [CH]=C=C=C | Yes |
| C=[C]C + C=C=C=C ↔ C=CC + [CH]=C=C=C | Yes |
| C=CC + [CH]=C=C=C ↔ C=C=C=C + [CH2]C=C | Yes |
| C=C=C + [CH]=C=C=C ↔ C=C=C=C + [CH]=C=C | No |
| C#CC + [CH]=C=C=C ↔ C=C=C=C + C#C[CH2] | No |
| [CH]=CC#C + C=C=C=C ↔ C#CC=C + [CH]=C=C=C | No |
| C#C[C]=C + C=C=C=C ↔ C#CC=C + [CH]=C=C=C | Yes |
| [CH]=CC=C + C=C=C=C ↔ C=CC=C + [CH]=C=C=C | Yes |
| C=[C]C=C + C=C=C=C ↔ C=CC=C + [CH]=C=C=C | Yes |
| CC=C=O + [CH]=C=C=C ↔ C=C=C=C + [CH2]C=C=O | Yes |
| C=CC=CC + [CH]=C=C=C ↔ C=C=C=C + [CH2]C=CC=C | No |
| [C]1=CCC=C1 + C=C=C=C ↔ C1=CCC=C1 + [CH]=C=C=C | No |
| C1=CCC=C1 + [CH]=C=C=C ↔ C=C=C=C + [CH]1C=CC=C1 | Yes |
| [c]1ccccc1 + C=C=C=C ↔ c1ccccc1 + [CH]=C=C=C | No |
| C1=CCCC=C1 + [CH]=C=C=C ↔ C=C=C=C + [CH]1C=CC=CC1 | Yes |
| C[CH]C(=O)C(C)C + C=C=C=C ↔ CCC(=O)C(C)C + [CH]=C=C=C | No |
| [OH] + C=C=C=C ↔ O + [CH]=C=C=C | Yes |
| [O]O + [CH]=C=C=C ↔ C=C=C=C + [O][O] | Yes |
| OO + [CH]=C=C=C ↔ C=C=C=C + [O]O | No |
| C=C1C=CCC1 + [CH]=C=C=C ↔ C=C=C=C + C=C1C=C[CH]C1 | No |
| C=C1C=CCC1 + [CH]=C=C=C ↔ C=C=C=C + C=C1[CH]CC=C1 | No |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C1CC=CC1 + [CH]=C=C=C ↔ C=C=C=C + C=C1[CH]C=CC1 | No |
| [CH]=C=O + C=C=C=C ↔ C=C=O + [CH]=C=C=C | Yes |
| C=O + [CH]=C=C=C ↔ C=C=C=C + [CH]=O | Yes |
| [CH2]O + C=C=C=C ↔ CO + [CH]=C=C=C | No |
| [CH2]CO + C=C=C=C ↔ CCO + [CH]=C=C=C | Yes |
| C[CH]O + C=C=C=C ↔ CCO + [CH]=C=C=C | Yes |
| CC[O] + C=C=C=C ↔ CCO + [CH]=C=C=C | Yes |
| [CH2]C=O + C=C=C=C ↔ CC=O + [CH]=C=C=C | Yes |
| CC=O + [CH]=C=C=C ↔ C=C=C=C + C[C]=O | Yes |
| C[CH2] + C=C=C=C ↔ CC + [CH]=C=C=C | Yes |
| [CH2]CC + C=C=C=C ↔ CCC + [CH]=C=C=C | No |
| C[CH]C + C=C=C=C ↔ CCC + [CH]=C=C=C | Yes |
| C=CC=O + [CH]=C=C=C ↔ C=C=C=C + C=C[C]=O | Yes |
| C=CCC + [CH]=C=C=C ↔ C=C=C=C + C=C[CH]C | Yes |
| C=C=C=C + [O] ↔ [OH] + [CH]=C=C=C | Yes |
| C=C=C=C + [CH2] ↔ [CH3] + [CH]=C=C=C | Yes |
| C=CCC + [CH3] ↔ C + [CH2]CC=C | Yes |
| [CH2]CC=C + C=CC ↔ C=CCC + [CH2]C=C | Yes |
| [CH2]CC=C + CC(C)C(=O)C(C)C ↔ C=CCC + C[C](C)C(=O)C(C)C | Yes |
| [CH2]CC=C + CC(C)C(=O)C(C)C ↔ C=CCC + [CH2]C(C)C(=O)C(C)C | No |
| [CH2]CC=C + C=CC=CC ↔ C=CCC + [CH2]C=CC=C | Yes |
| [CH2]CC=C + C1=CCCC=C1 ↔ C=CCC + [CH]1C=CC=CC1 | Yes |
| C=CCC + [H] ↔ [H][H] + [CH2]CC=C | No |
| C=CCC + [O] ↔ [OH] + [CH2]CC=C | Yes |
| C=CCC + [OH] ↔ O + [CH2]CC=C | Yes |
| [CH2]CC=C + [O]O ↔ C=CCC + [O][O] | No |
| [CH2]CC=C + OO ↔ C=CCC + [O]O | No |
| [CH2]CC=C + C#CC ↔ C=CCC + C#C[CH2] | No |
| [CH2]CC=C + C=C=C ↔ C=CCC + [CH]=C=C | Yes |
| C=CCC + [c]1ccccc1 ↔ c1ccccc1 + [CH2]CC=C | Yes |
| [CH2]CC=C + C=CC=C ↔ C=CCC + C=[C]C=C | Yes |
| [CH2]CC=C + C=C1C=CCC1 ↔ C=CCC + C=C1[CH]CC=C1 | No |
| [CH2]CC=C + C=C1CC=CC1 ↔ C=CCC + C=C1[CH]C=CC1 | No |
| [CH2]CC=C + C=C1C=CCC1 ↔ C=CCC + C=C1C=C[CH]C1 | No |
| C=CCC + [CH]=C ↔ C=C + [CH2]CC=C | Yes |
| C=CCC + [CH]=CC ↔ C=CC + [CH2]CC=C | Yes |
| C=CCC + C=[C]C ↔ C=CC + [CH2]CC=C | Yes |
| [CH2]CC=C + CCC ↔ C=CCC + [CH2]CC | Yes |
| [CH2]CC=C + CCC ↔ C=CCC + C[CH]C | Yes |
| C=CCC + [CH2] ↔ [CH3] + [CH2]CC=C | Yes |
| [CH2]CC=C + CCO ↔ C=CCC + C[CH]O | No |
| C=CCC + [CH2]CO ↔ CCO + [CH2]CC=C | Yes |
| C=CCC + CC[O] ↔ CCO + [CH2]CC=C | Yes |
| [CH2]CC=C + CC=O ↔ C=CCC + C[C]=O | Yes |
| [CH2]CC=C + CC=O ↔ C=CCC + [CH2]C=O | Yes |
| [CH2]CC=C + CC ↔ C=CCC + C[CH2] | Yes |
| C=CCC + [CH]=C=O ↔ C=C=O + [CH2]CC=C | Yes |
| [CH2]CC=C + CO ↔ C=CCC + [CH2]O | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=CCC + [C]#C ↔ C#C + [CH2]CC=C | Yes |
| [CH2]CC=C + C=O ↔ C=CCC + [CH]=O | No |
| [CH2]CC=C + CC=C=O ↔ C=CCC + [CH2]C=C=O | No |
| [CH2]CC=C + C=CC=O ↔ C=CCC + C=C[C]=O | Yes |
| C=CCC + [CH]=CC#C ↔ C#CC=C + [CH2]CC=C | Yes |
| [CH2]CC=C + C#CC=C ↔ C=CCC + C#C[C]=C | Yes |
| [CH2]CC=C + C=C=C=C ↔ C=CCC + [CH]=C=C=C | Yes |
| C=CCC + [CH]=CC=C ↔ C=CC=C + [CH2]CC=C | Yes |
| [CH2]CC=C + CCC(=O)C(C)C ↔ C=CCC + C[CH]C(=O)C(C)C | Yes |
| [CH2]CC=C + C=CCC ↔ C=CCC + C=C[CH]C | Yes |
| [CH2]CC=C + C1=CCC=C1 ↔ C=CCC + [CH]1C=CC=C1 | Yes |
| C=CCC + [C]1=CCC=C1 ↔ C1=CCC=C1 + [CH2]CC=C | Yes |
| CC(C)C + [CH3] ↔ C + [CH2]C(C)C | Yes |
| [CH2]C(C)C + C=CC ↔ CC(C)C + [CH2]C=C | Yes |
| [CH2]C(C)C + CC(C)C(=O)C(C)C ↔ CC(C)C + C[C](C)C(=O)C(C)C | Yes |
| [CH2]C(C)C + CC(C)C(=O)C(C)C ↔ CC(C)C + [CH2]C(C)C(=O)C(C)C | No |
| [CH2]C(C)C + C=CC=CC ↔ CC(C)C + [CH2]C=CC=C | Yes |
| [CH2]C(C)C + C1=CCCC=C1 ↔ CC(C)C + [CH]1C=CC=CC1 | Yes |
| CC(C)C + [H] ↔ [H][H] + [CH2]C(C)C | Yes |
| CC(C)C + [O] ↔ [OH] + [CH2]C(C)C | Yes |
| CC(C)C + [OH] ↔ O + [CH2]C(C)C | Yes |
| [CH2]C(C)C + [O]O ↔ CC(C)C + [O][O] | No |
| [CH2]C(C)C + OO ↔ CC(C)C + [O]O | No |
| [CH2]C(C)C + C#CC ↔ CC(C)C + C#C[CH2] | Yes |
| [CH2]C(C)C + C=C=C ↔ CC(C)C + [CH]=C=C | Yes |
| CC(C)C + [c]1ccccc1 ↔ c1ccccc1 + [CH2]C(C)C | Yes |
| CC(C)C + C=[C]C=C ↔ C=CC=C + [CH2]C(C)C | No |
| [CH2]C(C)C + C=C1C=CCC1 ↔ CC(C)C + C=C1[CH]CC=C1 | No |
| [CH2]C(C)C + C=C1CC=CC1 ↔ CC(C)C + C=C1[CH]C=CC1 | Yes |
| [CH2]C(C)C + C=C1C=CCC1 ↔ CC(C)C + C=C1C=C[CH]C1 | Yes |
| CC(C)C + [CH]=C ↔ C=C + [CH2]C(C)C | No |
| CC(C)C + [CH]=CC ↔ C=CC + [CH2]C(C)C | Yes |
| CC(C)C + C=[C]C ↔ C=CC + [CH2]C(C)C | Yes |
| CC(C)C + [CH2]CC ↔ CCC + [CH2]C(C)C | Yes |
| [CH2]C(C)C + CCC ↔ CC(C)C + C[CH]C | Yes |
| CC(C)C + [CH2] ↔ [CH3] + [CH2]C(C)C | Yes |
| [CH2]C(C)C + CCO ↔ CC(C)C + C[CH]O | No |
| CC(C)C + [CH2]CO ↔ CCO + [CH2]C(C)C | Yes |
| CC(C)C + CC[O] ↔ CCO + [CH2]C(C)C | Yes |
| [CH2]C(C)C + CC=O ↔ CC(C)C + C[C]=O | Yes |
| [CH2]C(C)C + CC=O ↔ CC(C)C + [CH2]C=O | Yes |
| [CH2]C(C)C + CC ↔ CC(C)C + C[CH2] | Yes |
| CC(C)C + [CH]=C=O ↔ C=C=O + [CH2]C(C)C | Yes |
| [CH2]C(C)C + CO ↔ CC(C)C + [CH2]O | Yes |
| CC(C)C + [C]#C ↔ C#C + [CH2]C(C)C | Yes |
| [CH2]C(C)C + C=O ↔ CC(C)C + [CH]=O | No |
| [CH2]C(C)C + CC=C=O ↔ CC(C)C + [CH2]C=C=O | No |
| [CH2]C(C)C + C=CC=O ↔ CC(C)C + C=C[C]=O | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| CC(C)C + [CH]=CC#C ↔ C#CC=C + [CH2]C(C)C | Yes |
| CC(C)C + C#C[C]=C ↔ C#CC=C + [CH2]C(C)C | Yes |
| [CH2]C(C)C + C=C=C=C ↔ CC(C)C + [CH]=C=C=C | Yes |
| CC(C)C + [CH]=CC=C ↔ C=CC=C + [CH2]C(C)C | Yes |
| [CH2]C(C)C + CCC(=O)C(C)C ↔ CC(C)C + C[CH]C(=O)C(C)C | Yes |
| [CH2]C(C)C + C=CCC ↔ CC(C)C + C=C[CH]C | Yes |
| [CH2]C(C)C + C1=CCC=C1 ↔ CC(C)C + [CH]1C=CC=C1 | Yes |
| CC(C)C + [C]1=CCC=C1 ↔ C1=CCC=C1 + [CH2]C(C)C | Yes |
| CC(C)C + [CH2]CC=C ↔ C=CCC + [CH2]C(C)C | Yes |
| [CH2]C(C)C(=O)C(C)C + C=CCC=C ↔ CC(C)C(=O)C(C)C + C=C[CH]C=C | Yes |
| C[C](C)C(=O)C(C)C + C=CCC=C ↔ CC(C)C(=O)C(C)C + C=C[CH]C=C | Yes |
| [H] + C=CCC=C ↔ [H][H] + C=C[CH]C=C | Yes |
| [CH3] + C=CCC=C ↔ C + C=C[CH]C=C | Yes |
| [C]#C + C=CCC=C ↔ C#C + C=C[CH]C=C | Yes |
| [CH]=C + C=CCC=C ↔ C=C + C=C[CH]C=C | No |
| [CH]=CC + C=CCC=C ↔ C=CC + C=C[CH]C=C | No |
| C=[C]C + C=CCC=C ↔ C=CC + C=C[CH]C=C | Yes |
| [CH2]C=C + C=CCC=C ↔ C=CC + C=C[CH]C=C | No |
| [CH]=C=C + C=CCC=C ↔ C=C=C + C=C[CH]C=C | Yes |
| C#C[CH2] + C=CCC=C ↔ C#CC + C=C[CH]C=C | No |
| [CH]=CC#C + C=CCC=C ↔ C#CC=C + C=C[CH]C=C | Yes |
| C#C[C]=C + C=CCC=C ↔ C#CC=C + C=C[CH]C=C | Yes |
| [CH]=CC=C + C=CCC=C ↔ C=CC=C + C=C[CH]C=C | No |
| C=[C]C=C + C=CCC=C ↔ C=CC=C + C=C[CH]C=C | No |
| [CH2]C=C=O + C=CCC=C ↔ CC=C=O + C=C[CH]C=C | No |
| [CH2]C=CC=C + C=CCC=C ↔ C=CC=CC + C=C[CH]C=C | Yes |
| [C]1=CCC=C1 + C=CCC=C ↔ C1=CCC=C1 + C=C[CH]C=C | Yes |
| [CH]1C=CC=C1 + C=CCC=C ↔ C1=CCC=C1 + C=C[CH]C=C | Yes |
| [c]1ccccc1 + C=CCC=C ↔ c1ccccc1 + C=C[CH]C=C | Yes |
| [CH]1C=CC=CC1 + C=CCC=C ↔ C1=CCCC=C1 + C=C[CH]C=C | No |
| C[CH]C(=O)C(C)C + C=CCC=C ↔ CCC(=O)C(C)C + C=C[CH]C=C | Yes |
| [OH] + C=CCC=C ↔ O + C=C[CH]C=C | Yes |
| [O]O + C=C[CH]C=C ↔ C=CCC=C + [O][O] | No |
| [O]O + C=CCC=C ↔ OO + C=C[CH]C=C | No |
| C=C1C=C[CH]C1 + C=CCC=C ↔ C=C1C=CCC1 + C=C[CH]C=C | No |
| C=C1[CH]CC=C1 + C=CCC=C ↔ C=C1C=CCC1 + C=C[CH]C=C | Yes |
| C=C1CC=CC1 + C=C[CH]C=C ↔ C=CCC=C + C=C1[CH]C=CC1 | Yes |
| [CH]=C=O + C=CCC=C ↔ C=C=O + C=C[CH]C=C | Yes |
| [CH]=O + C=CCC=C ↔ C=O + C=C[CH]C=C | Yes |
| [CH2]O + C=CCC=C ↔ CO + C=C[CH]C=C | Yes |
| [CH2]CO + C=CCC=C ↔ CCO + C=C[CH]C=C | Yes |
| C[CH]O + C=CCC=C ↔ CCO + C=C[CH]C=C | Yes |
| CC[O] + C=CCC=C ↔ CCO + C=C[CH]C=C | Yes |
| [CH2]C=O + C=CCC=C ↔ CC=O + C=C[CH]C=C | Yes |
| C[C]=O + C=CCC=C ↔ CC=O + C=C[CH]C=C | No |
| C[CH2] + C=CCC=C ↔ CC + C=C[CH]C=C | Yes |
| [CH2]CC + C=CCC=C ↔ CCC + C=C[CH]C=C | No |
| C[CH]C + C=CCC=C ↔ CCC + C=C[CH]C=C | Yes |

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**Table 3 – continued from previous page**

| Reactions | Found |
|---|---|
| C=C[C]=O + C=CCC=C ↔ C=CC=O + C=C[CH]C=C | Yes |
| [CH2]C(C)C + C=CCC=C ↔ CC(C)C + C=C[CH]C=C | Yes |
| C=C[CH]C + C=CCC=C ↔ C=CCC + C=C[CH]C=C | Yes |
| [CH2]CC=C + C=CCC=C ↔ C=CCC + C=C[CH]C=C | Yes |
| [CH]=C=C=C + C=CCC=C ↔ C=C=C=C + C=C[CH]C=C | Yes |
| C=CCC=C + [O] ↔ [OH] + C=C[CH]C=C | No |
| C=CCC=C + [CH2] ↔ [CH3] + C=C[CH]C=C | No |