

Supplementary Materials

Complex Reaction Processes in Combustion Unraveled by Neural Network Based Molecular Dynamics Simulation

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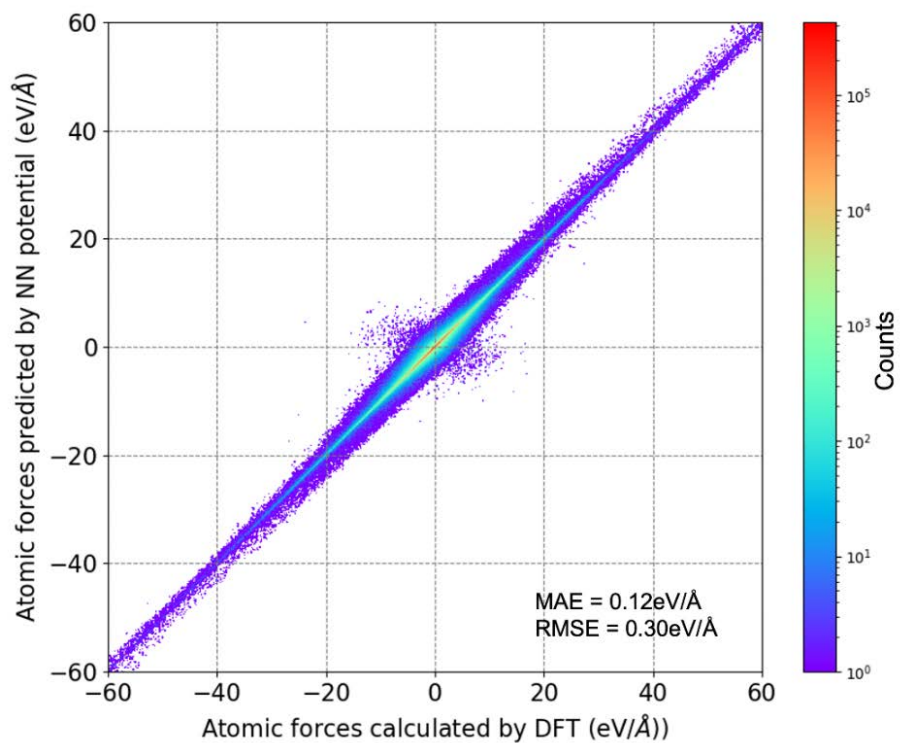


Figure 1. The correlation of atomic forces between NN predictions and DFT calculations. There are still a few points in the area with an absolute value greater than $60\text{eV}/\text{\AA}$. To make the picture clearer, they are not shown. However, these points were included when calculating the MAE and RMSE values. Considering such a large value range, the accuracy of the NN model is encouraging.

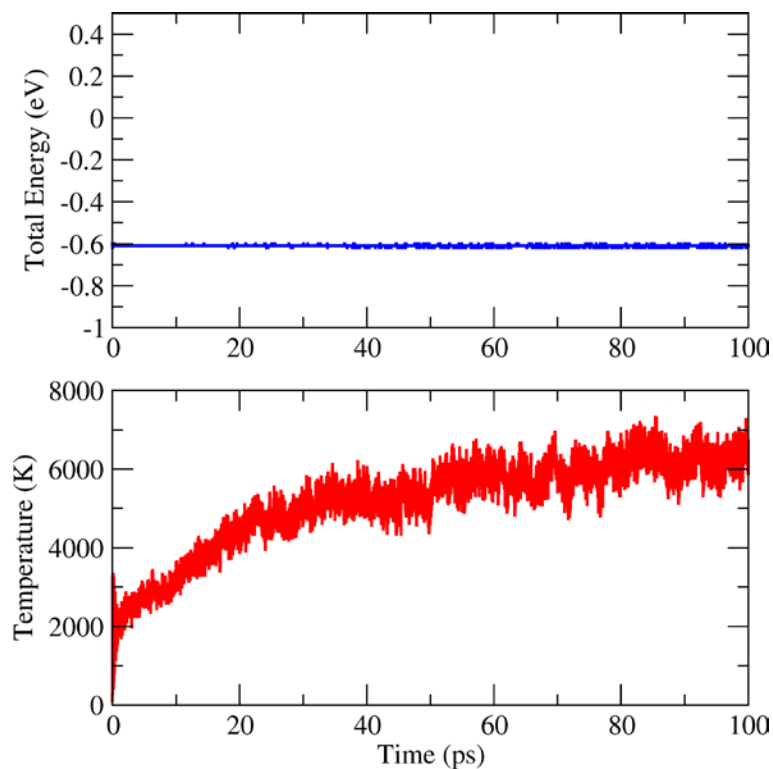


Figure 2. Time dependences of the total energy (the relative value to the first snapshot) and temperature during the MD simulation under NVE ensemble.

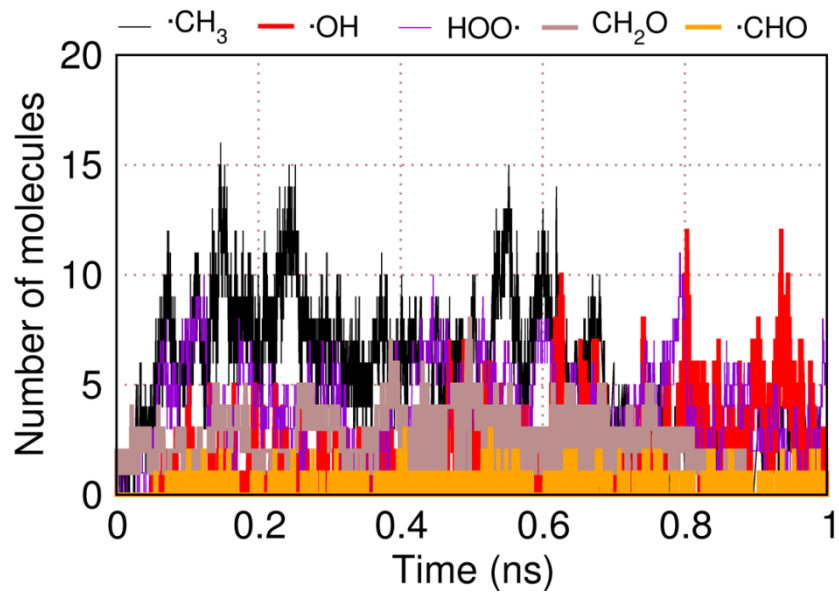


Figure 3. Time dependences of the numbers of main radicals created during the MD simulation.

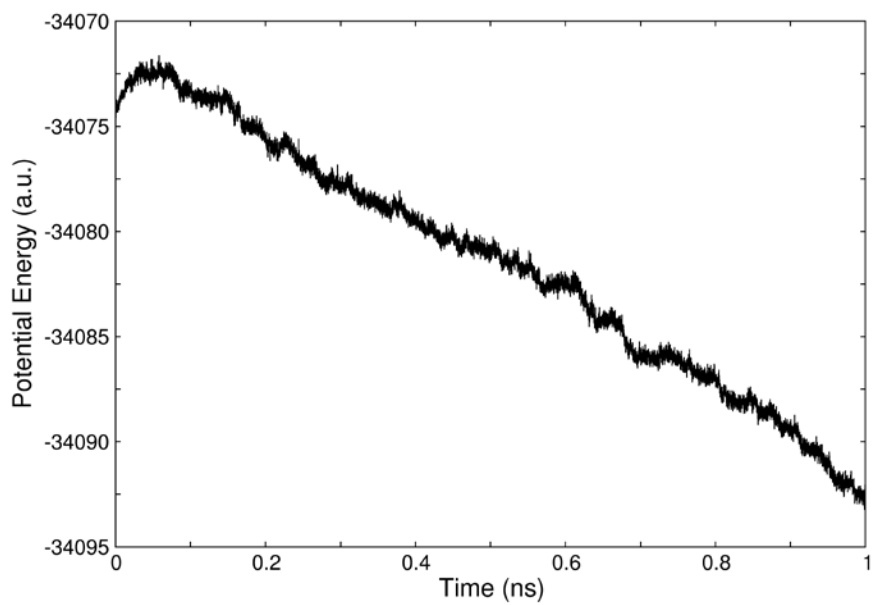


Figure 4. Time dependences of the potential energy of the system during the MD simulation.

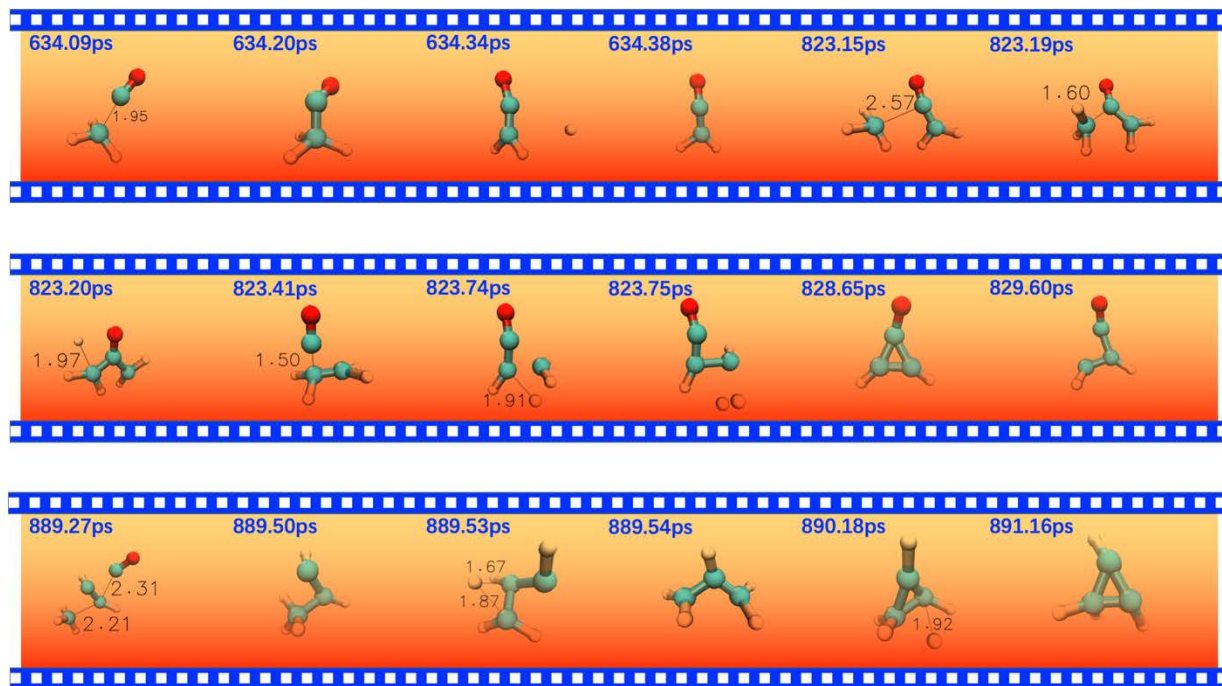


Figure 5. Real-time trajectory of the formation of cyclopropene.

Table 1. Energy prediction errors for the reference set. The mean absolute errors (MAEs) and root mean squared errors (RMSEs) are in eV/atom.

Training Set / Test Set		
Structure Number	MAE	RMSE
578,731 / 13,315	0.041 / 0.140	0.073 / 0.240

Table 2. Rate constants [(cm³/mol)·s⁻¹] of several reactions detected in the reactive MD simulation with neural network potential and comparison with that in the GRI-Mech 3.0 mechanism.

Reaction	$k(\text{exp})^{\text{a}}$	$k(\text{simulation})^{\text{b}}$
$\text{CH}_4 + \cdot\text{OH} \rightarrow \cdot\text{CH}_3 + \text{H}_2\text{O}$	2.17×10^{13}	1.22×10^{14}
$\cdot\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \cdot\text{OH}$	4.56×10^{11}	1.49×10^{13}
$\text{CH}_4 + \cdot\text{H} \rightarrow \cdot\text{CH}_3 + \text{H}_2$	4.60×10^{13}	4.34×10^{14}
$\cdot\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \cdot\text{H}$	2.92×10^{12}	8.49×10^{14}
$\cdot\text{CH}_3 + \text{HOO}\cdot \rightarrow \text{O}_2 + \text{CH}_4$	1.00×10^{12}	9.39×10^{13}
$\cdot\text{H} + \text{H}_2\text{O} \rightarrow \cdot\text{OH} + \text{H}_2$	7.17×10^{12}	6.57×10^{12}
$\text{CH}_4 + \text{HOO}\cdot \rightarrow \cdot\text{CH}_3 + \text{HOOH}$	1.89×10^{12}	4.79×10^{12}
$\cdot\text{O} + \text{CH}_4 \rightarrow \text{CH}_3 + \cdot\text{OH}$	3.96×10^{13}	8.05×10^{13}
$\text{O}_2 + \text{HOCO} \rightarrow \cdot\text{CHO} + \text{HOO}\cdot$	1.22×10^{11}	2.91×10^{12}
$\text{HOCO} + \cdot\text{OH} \rightarrow \cdot\text{CHO} + \text{H}_2\text{O}$	4.69×10^{13}	1.11×10^{14}

^aThe rate constants were calculated by the Arrhenius equation $k = AT^b e^{\frac{-E_a}{RT}}$, parameters are taken from Ref. 48, and T was set to 3000K.

^bThe rate constants were calculated by the method developed in Ref. 50 and Ref. 51.

Supplementary Note

List of reactions found in the trajectory

[HH]+[H]C([H])[H]->[H]C([H])([H])[H]
[HH]+[H]O->[H]O[H]
[HH]+[H]C[H]->[H]C([H])[H]
O=O->O+O
[H]C([H])=O->[HH]+[H]C=O
OO+[HH]->[H]OO
O+O->OO
[H]OC([H])([H])[H]->[HH]+[H]OC([H])[H]
O=O+[HH]->[H]OO
[H][H]->[HH]+[HH]
O=C=O->C=O+O
[H]C=O->C=O+[HH]
[H]C([H])([H])[H]+[H]O->[H]C([H])[H]+[H]O[H]
[HH]+[H]CO->[H]C([H])=O
[H]C([H])[H]+[H]O->[H]OC([H])([H])[H]
[H]C([H])O->[HH]+[H]C=O
[H]CO->C=O+[HH]
[HH]+[H]C([H])([H])[H]->[H]C([H])[H]+[H][H]
O+[HH]->[H]O
[HH]+[H]C([H])O->[H]C([H])([H])O
O+[H]O[H]->[H]O+[H]O
[H]C([H])([H])O->[HH]+[H]C([H])=O
C=O+O->O=CO
[H]OO[H]->[H]O+[H]O
[HH]+[H]CO->[H]C([H])O
O=O+[H]C([H])([H])[H]->[H]C([H])[H]+[H]OO
[H]C([H])[H]+[H]OO->OO+[H]C([H])([H])[H]
[H]O+[H][H]->[HH]+[H]O[H]
[H]O+[H]OO->O=O+[H]O[H]
[H]C([H])[H]+[H]O->[H]C[H]+[H]O[H]
[H]C([H])([H])[H]+[H]OO->[H]C([H])[H]+[H]OO[H]
OO+[H]O[H]->[H]O+[H]OO
[H]OC([H])([H])[H]->[HH]+[H]C([H])([H])O
[H]C([H])=O+[H]O->[H]C=O+[H]O[H]
OO+[H]C([H])=O->[H]C=O+[H]OO
[HH]+[H]OO->O+[H]O[H]
[H]OO+[H]O[H]->[H]O+[H]OO[H]
O+[H]C([H])([H])[H]->[H]C([H])[H]+[H]O
[HH]+[H]OO->O=O+[H][H]
O=O+[H]C([H])=O->[H]C=O+[H]OO
[H]C([H])=O+[H]O->[H]CO+[H]O[H]
OO+[H][H]->[HH]+[H]OO
[HH]+[H]C([H])[H]->[H]C[H]+[H][H]

$[H]C([H])([H])O + [H]O \rightarrow [H]C([H])O + [H]O[H]$
 $O=O + [H]C=O \rightarrow C=O + [H]OO$
 $[H]C([H])CO \rightarrow C=O + [H]C[H]$
 $[HH] + [H]C=O \rightarrow C=O + [H][H]$
 $[H]O + [H]OC([H])[H] \rightarrow [H]C([H])O + [H]O[H]$
 $O + [H]C([H])=O \rightarrow [H]C=O + [H]O$
 $O=O + [H]O \rightarrow O + [H]OO$
 $O=O + [H]C([H])([H])O \rightarrow [H]C([H])O + [H]OO$
 $[HH] + [H]OC([H])[H] \rightarrow [H]C([H])=O + [H][H]$
 $O + [H]C[H] \rightarrow [HH] + [H]CO$
 $O + [H]C([H])([H])O \rightarrow [H]C([H])=O + [H]O$
 $O + [H]C([H])[H] \rightarrow [HH] + [H]C([H])O$
 $OO + [H]C([H])([H])O \rightarrow [H]C([H])O + [H]OO$
 $OO + [H]C([H])=O \rightarrow [H]CO + [H]O=O$
 $[H]CO + [H]O=O \rightarrow OO + [H]C([H])O$
 $[H]C([H])[H] + [H]C([H])[H] \rightarrow [H]C([H])([H])C([H])([H])[H]$
 $[HH] + [H]C([H])([H])O \rightarrow [H]C([H])O + [H][H]$
 $C=O + [H]C([H])[H] \rightarrow [HH] + [H]C([H])C=O$
 $O + [H]C([H])=O \rightarrow [H]CO + [H]O$
 $O=O + [H]C([H])([H])O \rightarrow [H]C([H])=O + [H]OO$
 $C=O + [H]C([H])([H])[H] \rightarrow [H]C([H])[H] + [H]C=O$
 $O + [H]O \rightarrow O=O + [HH]$
 $OO + [H]OC([H])[H] \rightarrow [H]C([H])O + [H]OO$
 $[HH] + [H]C=O \rightarrow O + [H]C[H]$
 $[HH] + [H]C([H])=C=O \rightarrow [H]C(=O)C([H])[H]$
 $[H]C(=O)C([H])[H] \rightarrow [HH] + [H]C([H])CO$
 $[H]C([H])([H])=O \rightarrow [HH] + [H]C([H])=O$
 $[H]C([H])([H])=O \rightarrow [HH] + [H]C([H])O$
 $CO + O \rightarrow O=CO$
 $C=O + [H]C([H])([H])[H] \rightarrow [H]C([H])[H] + [H]CO$
 $C=O + [H]C[H] \rightarrow [H]C([H])\#CO$
 $C=O + [H]O \rightarrow O=CO + [HH]$
 $OCO \rightarrow C=O + O$
 $[HH] + [H]CC([H])[H] \rightarrow [H]C([H])C([H])[H]$
 $[H]C([H])[H] + [H]O \rightarrow [H]O=C([H])([H])[H]$
 $[H]C=C=O + [H][H] \rightarrow [HH] + [H]C([H])=C=O$
 $C=O + [H]C \rightarrow [H]CCO$
 $[H]C=C=O \rightarrow C=O + [H]C$
 $C=O + [H]O[H] \rightarrow [H]C=O + [H]O$
 $C=O + [H]OO \rightarrow O=O + [H]CO$
 $[H]C([H])[H] + [H]O \rightarrow [HH] + [H]OC([H])[H]$
 $[H]OO \rightarrow O + [H]O$
 $[H]C([H])([H])[H] \rightarrow [HH] + [HH] + [H]C[H]$
 $C=O \rightarrow C + O$
 $[HH] + [H]O[H] \rightarrow [H]O([H])[H]$
 $[HH] + [H]OO \rightarrow [H]OO[H]$

$[H]CC([H])C=O \rightarrow C=O + [H]CC[H]$
 $[H]C([H])([H])OO \rightarrow [HH] + [H]C([H])OO$
 $C=O + [H]CC[H] \rightarrow [H]CC([H])=C=O$
 $[HH] + [H]C([H])=C=O \rightarrow [H]C([H])([H])CO$
 $[HH] + [H]C([H])CO \rightarrow [H]C([H])([H])CO$
 $[H]OC([H])[H] \rightarrow [HH] + [H]CO[H]$
 $C=O + C=O \rightarrow O=CCO$
 $[H]C([H])=C=O \rightarrow [HH] + [H]C=C=O$
 $[H]OC([H])[H] \rightarrow [H]C[H] + [H]O$
 $C=O + [H]O \rightarrow [H]OC=O$
 $C=O + [H]C([H])[H] \rightarrow [H]C([H])([H])C=O$
 $O + [HH] + [HH] \rightarrow [H]O[H]$
 $OO + [H]C([H])[H] \rightarrow [H]C([H])([H])OO$
 $[HH] + [H]C=C=O \rightarrow [H]C([H])CO$
 $[H]CC([H])CO \rightarrow C=O + [H]CC[H]$
 $O=C=O + [HH] \rightarrow [H]OCO$
 $O=O + O=O \rightarrow OOOO$
 $OOOO \rightarrow O=O + OO$
 $[H]OO[H] \rightarrow O + [H]O[H]$
 $[H]C([H])([H])CO \rightarrow [HH] + [H]C([H])C=O$
 $[HH] + [H]CCO \rightarrow [H]C([H])CO$
 $[H]C([H])([H])C=O \rightarrow [HH] + [H]C([H])=C=O$
 $OOO \rightarrow O + OO$
 $[H]C([H])([H])C=O \rightarrow [HH] + [H]C([H])CO$
 $C=O + [H]O \rightarrow [H]OCO$
 $OOO \rightarrow O + O=O$
 $O + [H]C[H] \rightarrow [H]C([H])=O$
 $[H]C([H])C=O \rightarrow [HH] + [H]C=C=O$
 $[H]OC=O \rightarrow O=C=O + [HH]$
 $[H]C([H])=C=O \rightarrow [HH] + [H]CCO$
 $[HH] + [H]C([H])C=O \rightarrow [H]C([H])([H])C=O$
 $C=O + O=O \rightarrow O=COO$
 $O=C=O + OO \rightarrow O=C(O)OO$
 $[H]OCO \rightarrow O=CO + [HH]$
 $C=O + OO \rightarrow O=COO$
 $[H]C[H] \rightarrow [HH] + [H]C$
 $[HH] + [H]CC=O \rightarrow [H]C([H])C=O$
 $O=O + [H]C([H])[H] \rightarrow [H]C([H])([H])OO$
 $C=O + OO \rightarrow OCOO$
 $O=C=O + O=O \rightarrow O=C(O)OO$
 $[H]O + [H]O[H] \rightarrow [H]O[H]O[H]$
 $[H]C([H])([H])CO \rightarrow C=O + [H]C([H])[H]$
 $C=O + [H]C#C[H] \rightarrow [H]CC([H])C=O$
 $[H]O[H]C([H])([H])[H] \rightarrow [H]C([H])[H] + [H]O[H]$
 $[H]OC=O \rightarrow O=CO + [HH]$
 $[HH] + [H]CCO \rightarrow [H]C([H])C=O$

[H]C([H])CO->[HH]+[H]CC=O
 OCOO->C=O+O=O
 O=C(O)O->O+O=C=O
 [H]O[H]OO->O=O+[H]O[H]
 [H]C([H])=C=O->[HH]+[H]CC=O
 OOOO->OO+OO
 [H]C([H])([H])OO->O+[H]C([H])([H])O
 C=O+C=O->OCCO
 [H]CO[H]->[HH]+[H]OC
 OO+[H]O[H]->[H]O[H]OO
 OO+[H]O->[H]OOO
 O=CC=O->C=O+C=O
 [H]OC(=O)O->O=CO+[H]O
 C=O+[H]C#C[H]->[H]CC([H])=C=O
 [HH]+[H]CC([H])C([H])[H]->[H]C([H])C([H])C([H])[H]
 [HH]+[HH]+[H]C->[H]C([H])[H]
 [H]C(=O)O->O=CO+[HH]
 [H]C([H])([H])[H]+[H]O->[H]O[H]C([H])([H])[H]
 [H]C([H])[H]+[H]OO->[H]OOC([H])([H])[H]
 [H]OC([H])([H])O[H]->[H]O+[H]OC([H])[H]
 O=O+[H]C([H])([H])[H]->[H]C([H])([H])[H]OO
 [H]C([H])O->O+[H]C[H]
 O=C(O)OO->O=CO+OO
 [H]C([H])=C=O->[HH]+[H]C#CO
 C=O+[H]C=C[H]->[H]CC([H])C=O
 [H]O+[H]OC([H])[H]->[H]CO[H]+[H]O[H]
 O=O+[H]C([H])[H]->[H]C[H]+[H]OO
 O=C(O)O->O+O=CO
 [H]OOO->O=O+[H]O
 [H]OC([H])=O->[HH]+[H]OC=O
 [H]C([H])([H])[H]->[HH]+[HH]+[HH]+[H]C
 [H]OOC([H])([H])[H]->[H]C([H])([H])O+[H]O
 [H]OC([H])([H])[H]+[H]OO->[H]OC([H])[H]+[H]OO[H]
 [HH]+[H]O[H]->[H][H]O[H]
 O=O+[H]OC([H])[H]->[H]CO[H]+[H]OO
 [H]OC(=O)O->O=C=O+[H]O
 C=O+[H]C([H])C([H])[H]->[H]C([H])C([H])([H])C=O
 [H]C=C([H])C=O->C=O+[H]CC[H]
 C=O+O=C=O->O=COCO
 [H]C([H])C([H])C([H])[H]->[HH]+[H]C([H])CC([H])[H]
 [H]C1C([H])([H])C1([H])[H]->[HH]+[H]CC([H])C([H])[H]
 [H]C([H])([H])[H]OO->OO+[H]C([H])([H])[H]
 O=CO+[HH]->[H]C(O)O
 O1OO1->O+OO
 [H]C[H]+[H][H]->[H]C([H])([H])[H]
 [H]C1([H])[H][H]1->[HH]+[H]C([H])[H]

$O=C=O+O=O \rightarrow O=C(O)OO$
 $[H]C(=O)O \rightarrow O=C=O+[HH]$
 $OO[H]OO \rightarrow O=O+[H]OO$
 $[H]C([H])C(=O)C([H])([H])[H] \rightarrow [H]C([H])C=O+[H]C([H])[H]$
 $O=C(O)OCO \rightarrow O=C=O+O=C=O$
 $[H]OC([H])([H])O \rightarrow [HH]+[H]OC([H])O$
 $[H]OC([H])([H])O \rightarrow [HH]+[H]OC([H])=O$
 $[H]C([H])[H]+[H]O[H] \rightarrow [HH]+[H]OC([H])([H])[H]$
 $C=O+[HH] \rightarrow [H]OC$
 $[H]CC([H])CO \rightarrow C=O+[H]C\#C[H]$
 $[H]CC([H])([H])C=O \rightarrow [HH]+[H]CC([H])CO$
 $[HH]+[H]C1C([H])C1([H])[H] \rightarrow [H]C1C([H])([H])C1([H])[H]$
 $O=C=C(C=O)C=O+[H]O \rightarrow [H]OC(=O)C(=C=O)C=O$
 $[H]C([H])OO \rightarrow O+[H]C([H])=O$
 $[H]C([H])(O)O \rightarrow [HH]+[H]C(=O)O$
 $O+O=O \rightarrow O1OO1$
 $[H]OO[H] \rightarrow O+[HH]+[H]O$
 $[H]C[H]+[H]O \rightarrow [H]C([H])([H])O$
 $OCOO \rightarrow O+O=C=O$
 $[H][H]C([H])([H])[H] \rightarrow [HH]+[H]C([H])([H])[H]$
 $OO+[H]OO \rightarrow [H]OOOO$
 $[H]OOOO \rightarrow O=O+[H]OO$
 $[H]C[H]+[H]OO \rightarrow OO+[H]C([H])[H]$
 $[H]OOC([H])([H])[H] \rightarrow [HH]+[H]OOC([H])[H]$
 $[H]1[H]O1 \rightarrow [HH]+[H]O$
 $O+O+[HH] \rightarrow [H]OO$
 $O+O=CO \rightarrow O=COO$
 $O+O=CO \rightarrow OC(O)O$
 $O=C=O+O=O \rightarrow OOC(O)O$
 $[H]C([H])CO+[H]C([H])[H] \rightarrow [H]C([H])([H])C([H])([H])CO$
 $O=C=O+O=CO \rightarrow O=C(O)OCO$
 $[H]C([H])C(O)C([H])([H])[H] \rightarrow [H]C([H])C=O+[H]C([H])[H]$
 $[H]OOC(=O)O \rightarrow O=CO+[H]OO$
 $C=O+O=CO \rightarrow OCOCO$
 $[H]CO[H]+[H]OO \rightarrow OO+[H]OC([H])[H]$
 $[H]O[H]O \rightarrow [H]O+[H]O$
 $[H]C([H])([H])[H]+[H]O \rightarrow [HH]+[H]OC([H])([H])[H]$
 $[H]O[H]O \rightarrow O+[H]O[H]$
 $[H]OC([H])([H])CO \rightarrow [HH]+[H]OC([H])=C=O$
 $OCOCO \rightarrow C=O+O=C=O$
 $[H]C([H])CO+[H]O \rightarrow [H]OC([H])([H])CO$
 $[HH]+[H]C\#CO \rightarrow [H]C([H])C=O$
 $[H]OC([H])([H])CO \rightarrow [H]C([H])=C=O+[H]O$
 $C=O+[H]C([H])C([H])[H] \rightarrow [H]C([H])C([H])([H])CO$
 $[H]C([H])C([H])([H])CO \rightarrow [HH]+[H]C([H])C([H])CO$
 $[H]C1([H])C(=O)C1([H])[H] \rightarrow C=O+[H]C([H])C([H])[H]$

$[H]C1([H])C(=O)C1([H])[H] \rightarrow [HH] + [H]C1C(=O)C1([H])[H]$
 $O=CO + [H][H] \rightarrow [HH] + [H]C(=O)O$
 $[H]CC([H])=C=O \rightarrow C=O + [H]C=C[H]$
 $C=O + [H]CC([H])[H] \rightarrow [H]CC([H])([H])C=O$
 $[HH] + [H]CC([H])CO \rightarrow C=O + [H]CC([H])[H]$
 $C=O + [H]CC([H])[H] \rightarrow [H]C(=C=O)C([H])[H]$
 $[H]C([H])C([H])C([H])[H] \rightarrow [HH] + [H]C1C([H])C1([H])[H]$
 $[H]CCC([H])[H] \rightarrow [HH] + [H]CCC[H]$
 $[H]OC(=O)C(C=O)CO \rightarrow O=CC(C=O)CO + [H]O$
 $[H]OC([H])([H])O[H] \rightarrow [HH] + [H]OC([H])O[H]$
 $O=COO \rightarrow O+O=C=O$
 $OO + [H]CO[H] \rightarrow [H]CO + [H]OO$
 $[H]C([H])=O \rightarrow C=O + [HH] + [HH]$
 $[H]C([H])([H])[H] + [H]OO \rightarrow O + [H]C([H])[H] + [H]O[H]$
 $O=CO=O \rightarrow C=O + OO$
 $[H]OC([H])([H])[H] \rightarrow O + [H]C([H])([H])[H]$
 $O + [H]C([H])([H])[H] \rightarrow [HH] + [H]C([H])([H])O$
 $[H]C([H])[H] + [H]OC([H])[H] \rightarrow [H]C([H])([H])[H] + [H]CO[H]$
 $OOC1(O)OO1 \rightarrow O=C1OO1 + O=O$
 $O=C1OO1 + OO \rightarrow OOC1(O)OO1$
 $OO + [H]OC([H])([H])[H] \rightarrow [H]C([H])([H])O + [H]OO$
 $OO + [H]C([H])[H] \rightarrow [H]C([H])([H])O=O$
 $[HH] + [H]OOC([H])[H] \rightarrow [H]C([H])([H])O + [H]O$
 $[H]C([H])([H])[H] + [H]O \rightarrow [HH] + [H]C[H] + [H]O[H]$
 $O + [H]O \rightarrow [H]1OO1$
 $O=CO + OO \rightarrow OCOOO$
 $[H]C([H])[H] + [H]OO[H] \rightarrow [H]O + [H]OC([H])([H])[H]$
 $[H]C=O \rightarrow O + [H]C$
 $[H]C([H])=C=O + [H]C([H])[H] \rightarrow [H]C([H])C(=O)C([H])([H])[H]$
 $[H]C([H])([H])C([H])([H])CO \rightarrow [H]C([H])C=O + [H]C([H])[H]$
 $[H]C([H])C(=O)C([H])([H])[H] \rightarrow [HH] + [H]C([H])C(=O)C([H])[H]$
 $O=O + [H]C(=O)O \rightarrow O=CO + [H]OO$
 $O + [H]O \rightarrow [H]O=O$
 $O=O + [H]O([H])[H] \rightarrow [H]OO + [H]O[H]$
 $O=CO + [H]C([H])[H] \rightarrow [H]C([H])([H])C(=O)O$
 $OO + [H]OC([H])([H])[H] \rightarrow [H]OC([H])[H] + [H]OO$
 $OOC(O)O \rightarrow O=C=O + OO$
 $O + [H]O \rightarrow O[H]O$
 $[H]O + [H]OC=O \rightarrow [H]OC(=O)O[H]$
 $OOC(O)O \rightarrow O=CO + O=O$
 $O + [HH] + [H]C \rightarrow [H]C([H])=O$
 $[H]C([H])=C=O + [H]C([H])[H] \rightarrow [H]C([H])([H])C([H])([H])CO$
 $O=C=O + O=CO \rightarrow O=COC(=O)O$
 $[HH] + [H]OC([H])=C=O \rightarrow [H]OC([H])([H])C=O$
 $[H]OO + [H]O[H] \rightarrow [H]O + [H]O + [H]O$
 $[H]C([H])=O + [H]O \rightarrow [H]OC([H])([H])O$

[H]C([H])CO>[HH]+[H]C=CO
O=O+[H]C([H])=O>[H]C([H])(O)OO
O=O+[H]OC([H])([H])[H]>[H]OC([H])[H]+[H]OO
[H]O[H]+[H]O[H]>[H]O+[H]O([H])[H]
OO+[H]CO[H]>[H]OC+[H]OO
[HH]+[H]C1C(O)C1([H])[H]>[H]C1([H])C(=O)C1([H])[H]
[H]C([H])C([H])([H])C=O>[HH]+[H]C([H])C([H])C=O
[HH]+[H]C1C(=O)C1([H])[H]>[H]C([H])C([H])([H])CO
[H]CC([H])CO>C=O+[H]C=C[H]
[HH]+[H]CC([H])=C=O>[H]CC([H])([H])CO
[H]C([H])C([H])C=O>C=O+[H]CC([H])[H]
[H]C1C(O)C1([H])[H]>[HH]+[H]C1C([H])C1O
[H]C([H])C([H])C=O>[HH]+[H]CC([H])=C=O
[H]CC([H])([H])CO>C=O+[H]CC([H])[H]
[H]C([H])C([H])C=O>[HH]+[H]CC([H])CO
[H]CC([H])C(=O)O[H]>[H]CC[H]+[H]OCO
[H]CC[H]+[H]OC=O>[H]CC([H])C(=O)O[H]
[H]C(C=O)C([H])C([H])([H])[H]>C=O+[H]CC([H])C([H])([H])[H]
[H]C1C([H])([H])C1([H])[H]>[HH]+[H]C1([H])CC1([H])[H]
[HH]+[H]C1([H])CC1([H])[H]>[H]C([H])C([H])C([H])[H]
[HH]+[H]CC([H])C([H])[H]>[H]CC([H])([H])C([H])[H]
[H]CC([H])C([H])[H]>[HH]+[H]CC([H])C[H]
[HH]+[H]C1C([H])C1[H]>[H]CC([H])C([H])[H]
[H]C1C([H])C1[H]>[HH]+[H]C1CC1[H]
C=O+OCCCO>OCC(CO)CO
O=C=C(=C=O)=C=O>C=O+OCCCO
O=CC(CO)CO+[H]O>[H]OC(=O)C(=C=O)C=O
[H]OC(=O)C(CO)CO>O=CC(C=O)C=O+[H]O
O=C=C(=C=O)=C=O+[H]O>[H]OC(=O)C(=C=O)=C=O
[H]OC(O)C(=C=O)C=O>O=CC1C(O)C1O+[H]O
O=CC(C=O)CO+[H]O>[H]OC(O)C(C=O)CO
[H]OC(=O)C(=C=O)C=O>O=C=C(=C=O)C=O+[H]O
[H]OC([H])([H])O[H]>[HH]+[H]OC([H])([H])O
[HH]+[H]OC([H])([H])O>[H]OC([H])([H])O[H]2
[H]OC([H])O[H]+[H][H]>[HH]+[H]OC([H])([H])O[H]
OO+[H]O([H])[H]>[H]OO+[H]O[H]
[H]OC1(O)C(=O)C1=C=O>O=CC1C(=O)C1O+[H]O
[H]OC([H])O[H]>[H]CO[H]+[H]O
[H]OCO[H]+[H][H]>[HH]+[H]OC([H])O[H]
O=C=C(C=O)C=O+[H]O>[H]OC(O)C(=C=O)C=O
O=C=C(C=O)C(=O)O>O=CCC=O+O=CO
O=C=CC=O+O=CO>O=C=C(C=O)C(=O)O
O=CC(CO)C(=O)O>O=C=CC=O+O=CO
[H]C([H])([H])OO+[H]C([H])([H])[H]>[H]C([H])[H]+[H]OOC([H])([H])[H]
[H]C([H])([H])OO>[HH]+[H]C1([H])OO1
O+[H]C([H])=O>[H]C([H])(O)O

$O+[H]C(=O)O \rightarrow O=CO+[H]O$
 $[H]OOC([H])([H])[H] \rightarrow [HH]+[H]C([H])O+[H]O$
 $[H]OO+[H][H] \rightarrow O+[HH]+[H]O[H]$
 $[H]C([H])[H]+[H]O+[H]O \rightarrow [H]C([H])([H])[H]+[H]OO$
 $[H]C([H])=O+[H]OC([H])[H] \rightarrow [H]OC([H])([H])OC([H])[H]$
 $[H]C[H]+[H]O \rightarrow O+[H]C([H])[H]$
 $[H]O1[H]O1 \rightarrow [H]O+[H]O$
 $[H]CO[H]+[H]OC([H])[H] \rightarrow [H]OC([H])C([H])([H])O[H]$
 $[H]OO+[H]OO[H] \rightarrow O=O+[H]O+[H]O[H]$
 $[H]C1([H])([H])[H]O1 \rightarrow [H]C([H])[H]+[H]O$
 $[H]C([H])[H]+[H]OCO \rightarrow O=CO+[H]C([H])([H])[H]$
 $O+O=C=O \rightarrow O=C(=O)O$
 $O+OO \rightarrow O=OO$
 $C=O+OOO \rightarrow OC000$
 $[H]C([H])([H])[H]+[H]OC([H])([H])[H] \rightarrow [H]C([H])[H]+[H]C([H])[H]+[H]O[H]$
 $[H]C([H])[H]+[H]C([H])[H]+[H]O[H] \rightarrow [HH]+[H]C([H])([H])[H]+[H]OC([H])[H]$
 $O=O+[H]OO[H] \rightarrow [H]OO[H]OO$
 $[H]OC([H])[H]+[H]OO \rightarrow [H]CO[H]+[H]OO[H]$
 $OO+[H]CO[H] \rightarrow [H]OC([H])OO$
 $[H]OC([H])OO \rightarrow O+[H]OC([H])=O$
 $[H]OC([H])(O)O \rightarrow [H]O+[H]OCO$
 $[H]C([H])OO \rightarrow O+[H]C([H])O$
 $[H]CO+[H]O \rightarrow [H]OC([H])=O$
 $[H]OC([H])=O \rightarrow [HH]+[H]C(=O)O$
 $OO+[H]OO[H] \rightarrow [H]OO[H]OO$
 $[H]OC([H])([H])[H] \rightarrow [HH]+[H]C[H]+[H]O$
 $[H]C([H])[H]+[H]OC([H])[H] \rightarrow [H]C([H])([H])[H]+[H]C([H])O$
 $O=C1OO1+O=O \rightarrow O=OC1(O)OO1$
 $[H]OC([H])[H] \rightarrow [HH]+[HH]+[H]OC$
 $[H]C([H])([H])[H]+[H]OO \rightarrow O+[HH]+[H]C[H]+[H]O[H]$
 $O+[H]C[H]+[H]O[H] \rightarrow [H]C([H])[H]+[H]OO$
 $O=C=O \rightarrow C+O+O$
 $[H]C([H])OO \rightarrow [HH]+[H]C(O)O$
 $[HH]+[H]C(O)O \rightarrow [H]C([H])(O)O$
 $O=O+[H]OC=O \rightarrow O=C=O+[H]OO$
 $O=O+OO \rightarrow O=OOO$
 $[H]C([H])([H])OO+[H]C([H])=O \rightarrow [H]CO+[H]OOC([H])([H])[H]$
 $[H]C([H])([H])OO+[H]C([H])=O \rightarrow [H]C=O+[H]OOC([H])([H])[H]$
 $OO[H]OO \rightarrow OO+[H]OO$
 $[H]C([H])[H]+[H]OO \rightarrow [H]OO[H]C([H])[H]$
 $[H]C([H])([H])[H]+[H]C([H])[H] \rightarrow [H]C([H])([H])[H]C([H])([H])[H]$
 $OC000 \rightarrow O=C=O+OO$
 $O=C=O+[H]OO \rightarrow O=O+[H]OCO$
 $[H]C([H])=C=O \rightarrow O+[H]C([H])C$
 $[H]OO+[H]OO \rightarrow O+OO+[H]O[H]$
 $OO+[H]C([H])[H] \rightarrow [HH]+[H]C([H])OO$

$[H]C([H])O + [H]OO[H] \rightarrow [H]C=O + [H]O + [H]O[H]$
 $O=COO \rightarrow O + OCO$
 $O + OCO \rightarrow OC1OO1$
 $[H]C([H])[H] + [H]OO \rightarrow [H]C[H] + [H]OO[H]$
 $O=O + [H]C([H])O \rightarrow [H]C([H])(O)OO$
 $O=OC(=O)O \rightarrow O=C=O + OO$
 $[H]C([H])C(=O)C([H])([H])[H] \rightarrow [H]C([H])CO + [H]C([H])[H]$
 $[H]C([H])=C=O + [H]C([H])[H] \rightarrow [H]C([H])([H])C([H])([H])C=O$
 $O + [H]C([H])([H])O \rightarrow [HH] + [H]C([H])(O)O$
 $O=C=O + [H]OO \rightarrow [H]OOC(O)O$
 $[HH] + [H]C([H])=C=O \rightarrow [H]C([H])([H])=C=O$
 $[H]C([H])C=O + [H]C([H])[H] \rightarrow [H]C([H])=C(O)C([H])([H])[H]$
 $[H]C([H])=C(O)C([H])([H])[H] \rightarrow [H]C([H])=C=O + [H]C([H])[H]$
 $O=C=O + [H]C([H])([H])[H] \rightarrow [H]C([H])[H] + [H]OCO$
 $[H]C([H])([H])C(O)O \rightarrow O=CO + [H]C([H])[H]$
 $OCOO + [HH] \rightarrow [H]OOC=O$
 $[H]OOCO \rightarrow O=C=O + [H]O$
 $[H]O + [H]OO \rightarrow [H]O[H]OO$
 $O=CO + [H]C[H] \rightarrow [H]C([H])C(=O)O$
 $[H]C([H])(O)C=O \rightarrow C=O + [H]C([H])=O$
 $O + [H]C([H])([H])[H] + [H]O \rightarrow [H]C([H])[H] + [H]O[H]O$
 $[H]OC([H])[H] + [H]OO \rightarrow O + [H]OC([H])([H])O[H]$
 $O + [H]OC([H])([H])O[H] \rightarrow [H]O + [H]OC([H])([H])O$
 $[H]O + [H]OC([H])([H])O \rightarrow [H]OC([H])=O + [H]O[H]$
 $O + [H]C([H])([H])O \rightarrow [H]OC([H])([H])O$
 $[H]OC([H])([H])O \rightarrow [H]C=O + [H]O[H]$
 $[H]C=O + [H]O[H] \rightarrow [HH] + [H]OC([H])=O$
 $[H]OC([H])=O \rightarrow C=O + [H]O[H]$
 $C=O + [H]C=O \rightarrow [H]C(=O)OC$
 $[H]C(O)OC \rightarrow C=O + [H]C=O$
 $C=O + [H]C([H])=O \rightarrow [H]C([H])OCO$
 $[H]OC(O)O[H] \rightarrow [H]O + [H]OC=O$
 $[H]O + [H]OC=O \rightarrow O=C=O + [H]O[H]$
 $O=C=O + [H]OO \rightarrow [H]OOC(=O)=O$
 $[H]C([H])([H])C=O + [H]O \rightarrow [H]OC(=O)C([H])([H])[H]$
 $[H]OC(=O)C([H])([H])[H] \rightarrow [H]C([H])[H] + [H]OC=O$
 $C=O + OO \rightarrow O=OCO$
 $[H]OOOO \rightarrow OOO + [H]O$
 $C=O + [H]C([H])([H])O \rightarrow [H]C([H])=O + [H]CO$
 $[H]CO + [H]O[H] \rightarrow [H]C(O)O([H])[H]$
 $[H]C(=O)O([H])[H] \rightarrow [H]CO + [H]O[H]$
 $[H]O[H] \rightarrow O + [H][H]$
 $O=C=O + [H]C([H])[H] \rightarrow [H]C([H])([H])C(=O)O$
 $O=O + [H]O[H] \rightarrow [H]O([H])OO$
 $OO + [H]OCO \rightarrow [H]OC(=O)OO$
 $[H]OC(=O)OO \rightarrow O=O + [H]OCO$

OOO+[H]O[H]->[H]O+[H]OOO
 [H]OC([H])([H])[H]+[H]OO->[H]C([H])([H])O+[H]OO[H]
 OO+[H]OCO->O=CO+[H]OO
 [H]C([H])([H])O+[H]OC([H])[H]->[H]C([H])O+[H]OC([H])([H])[H]
 [H]C=O+[H]OO->C=O+[H]OO[H]
 [H]C=O+[H][H]->[H][H]C([H])=O
 [H][H]C([H])=O->[HH]+[H]C([H])=O
 OCCOO->O+O=CO
 C=O+O=CO->O=COC=O
 O=COC=O->C=O+O=C=O
 O=O+[H]C([H])[H]->[H]C[H]+[H]O=O
 C=O+[H]OO->[H]OOCO
 [H]OOC=O->C=O+[H]OO
 O+[H]C->[H]CO
 [H]C([H])[H]+[H]OO->O+[H]OC([H])([H])[H]
 O+[HH]+[H]C->[H]C([H])O
 [H]C([H])C([H])O->[HH]+[H]C([H])C=O
 O=C=O+O=O->OO=C(O)O
 OO=C(O)O->O=CO+OO
 C=O+[H]C([H])([H])OO->[H]C([H])([H])OOCO
 [H]C([H])([H])OOC=O->O=C=O+[H]C([H])([H])O
 [H]C([H])([H])C([H])([H])C=O->[H]C([H])C=O+[H]C([H])[H]
 OCO+[H][H]->[HH]+[H]C(O)O
 [HH]+[H]C(O)O->O=CO+[H][H]
 O+O=C=O->OC1OO1
 OOC(O)(O)O->O+O1OC12OO2
 O+O1OC12OO2->O=C(O)OOO
 O=C(O)OOO->O=C1OO1+O=O
 OO+[H]O[H]->[H]O([H])OO
 [H]C([H])CO+[H]C([H])[H]->[H]C([H])([H])C=O+[H]C[H]
 [H]C([H])([H])C=O+[H]C[H]->[H]C([H])([H])C([H])([H])CO
 [H]C([H])([H])CO->[HH]+[HH]+[H]C=C=O
 [H][H]C([H])[H]->[HH]+[H]C([H])[H]
 [H]C1([H])[H]O1->O+[H]C([H])[H]
 O+[H]C([H])[H]->[H]C([H])([H])O
 [H]OC([H])[H]->O+[HH]+[H]C[H]
 [HH]+[H]C+[H]O->[H]OC([H])[H]
 [H]C([H])C=O+[H]O->[H]OC([H])([H])CO
 [H]OC([H])([H])CO->C=O+[H]OC([H])[H]
 C=O+O=CO->O=COCO
 [H]O([H])[H]->[HH]+[HH]+[H]O
 O=C=O+[H]OO->OO+[H]OCO
 [H]C(=O)=O->O=CO+[HH]
 OO+[H]C([H])=O->[H]C(O)[H]OO
 [H]OOC(=O)O->O=C=O+[H]OO
 [H]C([H])[H]+[H][H]->[H][H]C([H])([H])[H]

$[H]C([H])[H]+[H]OO \rightarrow O=O+[H]C[H]+[H][H]$
 $O=C=O+[H]O \rightarrow [H]OC(O)O$
 $C=O+O=O \rightarrow COOO$
 $O=O+[H]OC([H])([H])O \rightarrow [H]O=C([H])O+[H]OO$
 $[H]OC([H])=O \rightarrow [H]C=O+[H]O$
 $[H]CO+[H]O \rightarrow [H]OC([H])O$
 $[H]O+[H]OC([H])=O \rightarrow [H]OC=O+[H]O[H]$
 $O=CO+[H]O[H] \rightarrow [H]O[H]OCO$
 $[H]O[H]+[H]O[H] \rightarrow [H]O[H]O([H])[H]$
 $O=CO+[H]O[H] \rightarrow [H]O([H])C(=O)O$
 $[H]O([H])C(=O)O \rightarrow O=C=O+[H]O[H]$
 $[H]O+[H]OO \rightarrow [H]OOO[H]$
 $OO+[H]OC([H])([H])[H] \rightarrow [H]C([H])([H])O[H]OO$
 $[H]C([H])([H])O[H]OO \rightarrow [H]C([H])([H])O+[H]OO$
 $[H]C([H])([H])O+[H]OO \rightarrow O=O+[H]OC([H])([H])[H]$
 $[HH]+[H]C=CO \rightarrow [H]C([H])=C=O$
 $C=O+[H]O[H] \rightarrow [H]O[H]CO$
 $[H]C([H])CO+[H]OC([H])[H] \rightarrow [H]OC([H])([H])C([H])([H])CO$
 $[H]OC([H])([H])C([H])([H])CO \rightarrow [H]C([H])=C=O+[H]OC([H])[H]$
 $OO+[H]OC([H])[H] \rightarrow [H]OC([H])([H])OO$
 $[H]OC([H])OO \rightarrow O=O+[H]CO[H]$
 $OO+[H]C=O \rightarrow [H]C(O)OO$
 $[H]C(=O)OO \rightarrow OO+[H]C=O$
 $[HH]+[H]CO \rightarrow [H]CO[H]$
 $[H]OC([H])([H])C=O \rightarrow [H]C([H])=C=O+[H]O$
 $[H]C([H])([H])O \rightarrow [HH]+[HH]+[H]C=O$
 $OO+[H][H] \rightarrow O+[H]O[H]$
 $OO+[H]C([H])C=O \rightarrow [H]C=C=O+[H]OO$
 $O=O+[H]OC([H])([H])[H] \rightarrow [H]C([H])([H])O[H]OO$
 $O=C=O+O=O \rightarrow OCOOO$
 $C=O+[H]O+[H]O \rightarrow OCO+[H]O[H]$
 $O=O+[H]OC \rightarrow [H]OCOO$
 $O=CO+[H]OO \rightarrow [H]OOC(O)O$
 $[HH]+[H]C#CO \rightarrow [H]C([H])CO$
 $O=O+[H]C[H] \rightarrow [H]C([H])OO$
 $[H]C1([H])OO1 \rightarrow [HH]+[H]C(O)O$
 $[H]O([H])O \rightarrow O+[H]O[H]$
 $[H]OC([H])([H])C=O \rightarrow C=O+[H]OC([H])[H]$
 $[H]C([H])O+[H]O \rightarrow [H]OC([H])([H])O$
 $[H]C([H])([H])[H]+[H]C([H])=C(O)C([H])[H] \rightarrow [H]C([H])[H]+[H]OC(C([H])[H])C([H])[H]$
 $[H]C([H])[H]+[H]OC(C([H])[H])C([H])[H] \rightarrow [H]C([H])([H])[H]+[H]C([H])C(O)C([H])[H]$
 $[H]C([H])C([H])([H])CO \rightarrow [HH]+[H]C([H])C([H])C=O$
 $[H]C([H])C([H])([H])C=O \rightarrow [HH]+[H]C1C(O)C1([H])[H]$
 $[HH]+[H]C([H])C([H])CO \rightarrow [H]C1([H])C(=O)C1([H])[H]$
 $[HH]+[H]C([H])C([H])C=O \rightarrow C=O+[H]C([H])C([H])[H]$
 $[H]C([H])C([H])([H])CO \rightarrow [HH]+[H]CC([H])([H])CO$

[H]C([H])C([H])([H])C=O->C=O+[HH]+[H]CC([H])[H]
C=O+[H]C([H])C([H])[H]->[H]C1([H])C(O)C1([H])[H]
[H]C1([H])C(O)C1([H])[H]->[HH]+[H]C1C(O)C1([H])[H]
[HH]+[H]C1C(O)C1([H])[H]->[H]C([H])C([H])([H])CO
[HH]+[H]C1C(=O)C1([H])[H]->C=O+[H]C([H])=C([H])[H]
C=O+[H]C([H])C([H])[H]->[HH]+[H]CC([H])([H])C=O
[H]C([H])C([H])([H])CO->C=O+[HH]+[H]CC([H])[H]
[H]C([H])C([H])([H])CO->[HH]+[H]C(=C=O)C([H])[H]
[HH]+[H]C(=C=O)C([H])[H]->[H]CC([H])=C=O+[H][H]
C=O+[H]O[H]->[H]O+[H]OC
[H]C([H])([H])O+[H]O[H]->[H]C([H])=O+[H]O([H])[H]
[H]C([H])O+[H]O([H])[H]->[H]C([H])([H])O+[H]O[H]
[H]C1C([H])C1O->C=O+[H]C=C[H]
[H]CC([H])=CO->C=O+[H]CC[H]
CO+[H]CC[H]->[H]CC([H])CO
C=O+[H]CC[H]->[H]C1C([H])C1O
C=O+[H]CC[H]->[H]C=C([H])CO
[HH]+[H]C(=O)O->O=C=O+[H][H]
O=O+OC1OO1->OOC1(O)OO1
O=C(O)O+[H]C([H])([H])[H]->[H]C([H])[H]+[H]OC(=O)O
[HH]+[H]CC([H])C=O->C=O+[H]CC([H])[H]
[H]CC([H])([H])CO->[HH]+[H]C1C(=O)C1[H]
C=O+O=C=O->COC(=O)O
[H]O+[H]O[H]->[H]OO([H])[H]
[HH]+[H]C1C(=O)C1[H]->[H]C1C(O)C1([H])[H]
[HH]+[H]C1C([H])C1O->[H]C1C(=O)C1([H])[H]
[HH]+[H]C1C([H])C1O->[H]CC([H])([H])C=O
[H]CC([H])([H])C=O->[H]C+[H]C([H])=C=O
[H]CC([H])([H])CO->[HH]+[H]CC([H])CO
[HH]+[H]CC([H])=C=O->[H]C([H])C([H])CO
C=O+[H]CC([H])[H]->[H]C1C(O)C1([H])[H]
[HH]+[H]CC([H])CO->[H]C(=C=O)C([H])[H]
[H]C([H])C([H])CO->C=O+[H]CC([H])[H]
[HH]+[H]CC([H])=C=O->[H]C(=C=O)C([H])[H]
[H]C([H])C([H])C=O->[HH]+[H]CC([H])C=O
[H]OC(=O)O[H]->[H]O+[H]OCO
[H]C=C([H])C=O->C=O+[H]C=C[H]
[H]C1C([H])C1O->[HH]+[H]C1CC1O
[HH]+[H]C1CC1O->[H]C1=C([H])C1O
[H]C1C(=O)C1[H]->O+[H]C1CC1[H]
[H]C([H])([H])O+[H]OO->[H]C([H])O+[H]O+[H]O
C=O+O=C=O->O=CC(=O)O
O=C=C(=O)O->C=O+O=C=O
[H]CC([H])CO+[H]O->[H]C(=C)C=O+[H]O[H]
[H]C(=C)C=O+[H]O[H]->[H]CC([H])C=O+[H]O
[H]CC([H])C=O+[H]O->[H]CC([H])C(=O)O[H]

[H]CC([H])C(=O)O[H]->[H]C=C[H]+[H]OC=O
[H]CC([H])C(O)O[H]->[H]CC[H]+[H]OC=O
[H]OC1(O)C([H])C1[H]->[H]CC[H]+[H]OC=O
[H]CC[H]+[H]OCO->C=O+[H]CC([H])O[H]
C=O+[H]CC([H])O[H]->[H]CC([H])C(=O)O[H]
[H]OC1(O)C([H])C1[H]->[H]C1C(=O)C1[H]+[H]O
[H]C1C([H])C1O+[H]O->[H]OC1([H])C([H])C1O
[H]C([H])C=O+[H]OO->[H]C([H])CO[H]OO
O=O+[H]C([H])CO[H]OO->OO[H]OO+[H]C([H])CO
[H]OC([H])C([H])C=O->C=O+[H]CC[H]+[H]O
C=O+[H]CC([H])C=O->[H]C(C=O)C([H])C=O
[H]C(=C=O)C([H])C=O->C=O+[H]CC([H])C=O
O=O+[H]C([H])=C=O->[H]C#CO+[H]OO
C=O+[H]CC[H]->[HH]+[H]CCC=O
[HH]+[H]CCC=O->[H]CC([H])C=O
[HH]+[H]CCC=O->[H]CC([H])CO
[H]CC([H])CO->C=O+[H]C+[H]C
C=O+[H]C+[H]C->[H]CC([H])C=O
[H]OCO->OCO+[HH]
[H]CC([H])O->[HH]+[H]CC=O
[HH]+[H]CCO->[H]CC([H])=O
[H]C1C([H])C1O+[H]OO->OO+[H]OC1C([H])C1[H]
[H]CC([H])=O->[HH]+[H]C=C=O
[H]C([H])CO+[H]OO->O=O+[H]C([H])([H])C=O
OO+[H]OC1C([H])C1[H]->[H]C1C(=O)C1[H]+[H]OO
[H]C1C(=O)C1[H]->C=O+[H]CC[H]
C=O+[H]C([H])[H]+[H]CC[H]->[H]C(C=O)C([H])C([H])([H])[H]
[H]CC([H])C([H])([H])[H]->[H]C([H])[H]+[H]CC[H]
[H]C([H])[H]+[H]CC([H])C=O->[H]C(C=O)C([H])C([H])([H])[H]
[H]CC([H])C([H])([H])[H]->[HH]+[H]CC([H])C([H])[H]
C=O+[H]CC([H])C([H])([H])[H]->[H]C(CO)C([H])C([H])([H])[H]
[H]C(CO)C([H])C([H])([H])[H]->[HH]+[H]C([H])C([H])C([H])C=O
[HH]+[H]C([H])C([H])C([H])C=O->[H]C([H])C([H])([H])C([H])C=O
[H]C([H])C([H])([H])C([H])C=O->[H]C(=C=O)C([H])[H]+[H]C[H]
[H]C(=C=O)C([H])[H]+[H]C[H]->C=O+[H]C([H])C([H])C([H])[H]
C=O+[HH]+[H]C([H])CC([H])[H]->[H]C([H])C([H])(C=O)C([H])[H]
[H]C([H])C(C=O)C([H])([H])[H]->C=O+[HH]+[H]C([H])CC([H])[H]
[HH]+[H]C([H])=CC([H])[H]->[H]C([H])CC([H])([H])[H]
[H]C([H])CC([H])([H])[H]->[HH]+[H]C([H])CC([H])[H]
[H]C1C([H])([H])C1([H])[H]->[HH]+[H]C([H])C([H])([H])C
C=O+[HH]+[H]C([H])C([H])([H])C->[H]C(=C=O)C([H])([H])C([H])[H]
[H]C(=C=O)C([H])([H])C([H])[H]->[H]C#CO+[H]C([H])C([H])[H]
[H]C([H])C([H])[H]+[H]C=C=O->[HH]+[H]C1([H])C(CO)C1([H])[H]
[HH]+[H]C1([H])C(CO)C1([H])[H]->[H]C1([H])C([H])([H])C1([H])CO
[H]C([H])C([H])(CO)C([H])[H]->C=O+[HH]+[H]C([H])CC([H])[H]
C=O+[H]C([H])=C([H])C([H])[H]->[HH]+[H]C([H])CC([H])([H])C=O

[HH]+[H]C([H])CC([H])([H])CO->[H]C(=O)C([H])C([H])C([H])[H]
[H]C(=O)C([H])C([H])C([H])[H]->C=O+[H]C([H])C([H])C([H])[H]
C=O+[H]C([H])C([H])C([H])[H]->[H]C([H])C([H])C([H])([H])CO
[H]C([H])C([H])C([H])([H])CO->C=O+[H]C=C([H])[H]+[H]C[H]
[H]CC([H])[H]+[H]C[H]->[H]C1C([H])([H])C1([H])[H]
[H]OOC=O->O=CO+[H]O
[HH]+[H]C1([H])CC1([H])[H]->[H]CC([H])([H])C([H])[H]
[HH]+[H]C([H])CC([H])[H]->[H]C1C([H])([H])C1([H])[H]
[H]C([H])C([H])C([H])[H]->[HH]+[HH]+[H]CCC([H])[H]
[H]CC([H])C([H])[H]->[H]C([H])C+[H]C[H]
[H]C1C([H])([H])C1([H])[H]->[HH]+[HH]+[H]C1CC1([H])[H]
O=O+[H]C1C([H])([H])C1([H])[H]->[H]CC([H])C([H])[H]+[H]OO
[H]CC([H])([H])C([H])[H]->[HH]+[H]C1C([H])C1([H])[H]
[HH]+[H]CC([H])C([H])[H]->[H]CC([H])C[H]+[H][H]
[H]C1C([H])C1[H]->[HH]+[H]CCC[H]
[H]C1CC1([H])[H]->[HH]+[H]C1CC1[H]
[HH]+[H]C1CC1[H]->[H]CCC([H])[H]
O+O=C=O->OC(O)O
[H]CC([H])C[H]->[HH]+[H]CCC[H]
[H]CCC[H]+[H]O[H]->[H]CC([H])C[H]+[H]O
[H]CCC[H]+[H]OO->OO+[H]CC([H])C[H]
C=O+[H]CCC([H])[H]->[HH]+[H]CCC([H])=C=O
[H]C=CC([H])=C=O->[HH]+[H]C#CCC=O
O=O+[H]CCC=C=O->[H]CCC(CO)OO
[H]CCC(CO)OO->OO+[H]CCC=C=O
OO+[H]CCCC=O->[H]C=CC(CO)OO
[H]CC(C=C=O)OO->OO+[H]CCC=C=O
OO+[H]CCC=C=O->[H]C(CCC=O)OO
[H]C(=O)C(O)CCO->CO+[H]C(=O)C1CO1
CO+[H]C(=O)C1CO1->[H]C(O)C1OC1CO
[H]C(O)C1OC1CO->O=CCCO+[H]CO
OC=CCO+[H]C=O->[H]C(O)C1OC1C=O
O=C=O+[H]C(O)C1OC1CO->[H]C(=O)CC(CO)OC(=O)O
[H]C(=O)CC(CO)OC(=O)O->O=C=O+[H]C(O)C1OC1C=O
[H]C(=O)C1OC1CO->OCC1CO1+[H]C=O
C=O+[H]C(O)C1OC1CO->[H]C(=O)C1OC1COOC
C=O+[H]C(O)C1OC1CO->[H]C(OCO)C1OC1CO
[H]C(OCO)C1OC1C=O->C=O+[H]C(=O)C1OC1CO
[H]C(OCO)C1OC1C=O->C=O+[H]C(O)C1OC1C=O
[H]C(=O)C(O)CCO->O=C=CC=O+[H]C=O
O=C=O+O=C=O->O=COC(=O)O
[H]C([H])[H]+[H]O->[HH]+[H]C1([H])[H]O1
[HH]+[H]C1([H])[H]O1->[H]OC([H])([H])[H]
[H]C([H])=O+[H]OO->O+[H]C=O+[H]O[H]
O=CC#CO+[H]C([H])=O->[H]C([H])(O)C(C=O)C=O
C=O+[H]C([H])(O)C(=C=O)C=O->[H]C([H])(OCO)C(=C=O)C=O

[H]C([H])(OCO)C(=C=O)C=O->O=C=CC=O+[H]C([H])OCO
O=C=CC=O+[H]C([H])OCO->C=O+[H]C([H])(O)C(=C=O)=C=O
[H]OC([H])O->[HH]+[H]C(O)O
[H]C([H])(O)C(C=O)CO->[HH]+[H]C(=O)C(C=O)CO
OO+[H]C(=O)C(=C=O)C=O->O=CC(C=O)CO+[H]OO
O=C=C(=C=O)=C=O+[HH]->[H]OCC(C=O)CO
[H]OCC(C=O)CO->O=C=C(C=O)CO+[HH]
O=C=C(C=O)C=O->C=O+OCCCO
OO+[H]OC=O->[H]OC(=O)OO
[H]OC(O)(O)O->O=C1OO1+[H]O
O=C(O)O+[H]C([H])([H])[H]->O=CO+[H]C([H])[H]+[H]O
OO+[HH]+[H]O[H]->[H]O+[H]OO[H]
[H]OC(=O)C(=C=O)C=O->O=C=C(=C=O)=C=O+[H]O
[H]O+[H]O[H]->[HH]+[H]O[H]O
[H]OC(=O)C(C=O)C=O->OCC(CO)CO+[H]O
OCC(CO)CO+[H]O->[H]OC1(O)C(O)C1C=O
[H]OC(=O)C(=C=O)C=O->O=C1C(O)C1CO+[H]O
O=CC(C=O)C=O+[H]O->[H]OC(=O)C(C=O)CO
O=C=C(C=O)CO+[H]O->[H]OC(=O)C(C=O)C=O
[H]OC(O)C(C=O)C=O->O=C=C(C=O)C=O+[H]O
[H]OC(=O)C(=C=O)C=O->O=C=C(=C=O)CO+[H]O
OCC(CO)CO+[H]O->[H]OC(=O)C(CO)CO
[H]OC(=O)C(=C=O)C=O->C=O+[H]OC(=O)CC=O
C=O+[H]OC(=O)CC=O->[H]OC1(O)C(=O)C1C=O
[H]OC1(O)C(O)C1CO->O=C=C(C=O)C=O+[H]O
O=CC(CO)CO+[H]O->[H]OC(=O)C(=C=O)CO
O=C=C(=C=O)C=O+[H]O->[H]OC(O)C(C=O)C=O
O=COC(=O)O->O=CO+O=CO
[H]OC(=O)C(CO)CO->O=C=C(=C=O)C=O+[H]O
[H]OC1(O)C(=O)C1CO->O=CC1C(=O)C1=O+[H]O
O=C1C(O)C1CO+[H]O->[H]OC1(O)C(=O)C1C=O
[H]OC(=O)C(CO)CO->O=CCCO+[H]OC=O
O=CCCO+[H]OC=O->[H]OC(=O)C(C=O)CO
[H]OC(=O)C(=C=O)C=O->O=C1CC1=O+[H]OC=O
O=C1CC1=O+[H]OC=O->[H]OC(=O)C(=C=O)=C=O
OO+[H]OC=O->O=CO+[H]OO
[H]OOC([H])([H])[H]->[H]O+[H]OC([H])[H]
[H]O=CO->O=CO+[HH]
O=C=C(=C=O)C=O->C=O+O=C=CC=O
C=O+OCCCO->O=CC1C(=O)C1O
O=C=C1C(=O)C1=O->C=O+OCCCO
O=CC(CO)CO->C=O+OCCCO
C=O+OCCCO->O=C1C(=O)C1CO
O=CC1C(=O)C1=O->C=O+O=C1CC1=O
C=O+O=C1CC1=O->O=C=C1C(=O)C1=O
O=C=C(=C=O)C=O->C=O+OCCCO

$O=CC(CO)CO+[H]O \rightarrow [H]OC1(O)C(=O)C1C=O$
 $[H]OC(=O)C(C=O)CO \rightarrow O=CC(CO)CO+[H]O$
 $O=C=C(C=O)CO+[H]O \rightarrow [H]OC1(O)C(=O)C1C=O$
 $[H]OC(=O)C(C=O)C=O \rightarrow O=CC(C=O)C=O+[H]O$
 $O=C=C(C=O)C=O+[H]O \rightarrow [H]OC1(O)C(=C=O)C1O$
 $O=CC(CO)CO \rightarrow C=O+O=C=C=C=O$
 $C=O+O=C1CC1O \rightarrow O=CC1C(=O)C1=O$
 $O=CC(CO)CO \rightarrow C=O+O=CCCO$
 $C=O+O=C1CC1O \rightarrow O=CC1C(=O)C1O$
 $O=CC1C(=O)C1O \rightarrow C=O+O=CCCO$
 $C=O+OCCCO \rightarrow O=CC(C=O)CO$
 $O=CC(C=O)CO \rightarrow C=O+O=CCCO$
 $C=O+O=CCCO \rightarrow O=C=C(=C=O)C=O$
 $[H]OC([H])O[H] \rightarrow [HH]+[H]OC([H])=O$
 $[H]O+[H]OC([H])O[H] \rightarrow [H]OCO[H]+[H]O[H]$
 $[H]OC1(O)C(=O)C1=C=O \rightarrow O=C=C(=C=O)C=O+[H]O$
 $O=C=C(C=O)C=O+O=CO \rightarrow O=CC(C=O)(CO)C(=O)O$
 $O=C(O)C1(CO)C(=O)C1=O \rightarrow O=C=C1C(=O)C1O+O=C=O$
 $[H]OC(=O)C(=C=O)=C=O \rightarrow O=C=C(=C=O)C=O+[H]O$
 $OO+[HH]+[HH] \rightarrow O+[H]O[H]$
 $O=CO+[H]OC1(O)C(=O)C1C=O \rightarrow [H]OC(=O)C(C=O)(C=O)C(=O)O$
 $[H]OC(=O)C(CO)(CO)C(=O)O \rightarrow O=CO+[H]OC(=O)C(=C=O)=C=O$
 $O=CO+[H]OC(=O)C(=C=O)=C=O \rightarrow [H]OC(=O)C(C=O)(CO)C(=O)O$
 $[H]OC(=O)C(CO)(CO)C(=O)O \rightarrow O=CO+[H]OC(=O)C(=C=O)C=O$
 $[H]OC(=O)C(CO)(CO)C(=O)O \rightarrow O=CO+[H]OC(=O)C(C=O)CO$
 $[H]OC(O)C(=C=O)C=O \rightarrow O=C=C(=C=O)C=O+[H]O$
 $[H]OC(=O)C(CO)CO \rightarrow O=CC(CO)CO+[H]O$
 $O=CC(CO)CO+[H]O \rightarrow [H]OC(=O)C(=C=O)=C=O$
 $O=O+[H]OC(=O)C(C=O)CO \rightarrow [H]OC(=O)C(CO)COOO$
 $[H]OC(=O)C(=C=O)COO=O \rightarrow OO+[H]OC(=O)C(=C=O)C=O$
 $[H]OC(=O)C(=C=O)=C=O \rightarrow O=C=C(C=O)C=O+[H]O$
 $O=C=C(=C=O)=C=O+[H]O \rightarrow [H]OC(=O)C(C=O)C=O$
 $O=C=O+[H]O[H] \rightarrow [H]O[H]OC=O$
 $[H]C([H])[H]+[H]OC(=O)C(=C=O)=C=O \rightarrow O=C=C(=C=O)C(=O)O+[H]C([H])([H])[H]$
 $O=CC(CO)C(=O)O \rightarrow O=C=C=C=O+O=CO$
 $O=C=C=C=O+O=CO \rightarrow O=C=C(C=O)C(=O)O$
 $O=CO+OCCCO \rightarrow O=C=C(C=O)C(=O)O$
 $O=CCCO+O=CO \rightarrow O=C(O)C(CO)CO$
 $O=C(O)C(CO)CO \rightarrow O=C=CC=O+O=CO$
 $O=CO+O=O \rightarrow O=C000$
 $O=C=CC=O+O=CO \rightarrow O=C=C(=C=O)C(=O)O$
 $O=C=C=C=O+O=CO \rightarrow O=C(O)C(CO)CO$
 $O=C(O)C(CO)CO \rightarrow O=C=O+OCCCO$
 $O=C=C=C=O+O=CO \rightarrow O=CC(C=O)C(=O)O$
 $O=CC(C=O)C(=O)O \rightarrow O=CCC=O+O=CO$
 $O=C=C(C=O)C(=O)O \rightarrow O=CCCO+O=CO$

[H]CO[H]+[H]O[H]->[H]OC([H])([H])O[H]
[H]C([H])(O)OO->OO+[H]C([H])O
C=O+O=O->C=OOO
[H]C[H]+[H]O[H]->[H]O[H]C([H])[H]
O=CCC=O->CCC=O+O
CCCCO+O->OCCCCO
O=CC(CO)C(=O)O->O=CCCCO+O=CO
O=CO+OCCCCO->O=CC(CO)C(=O)O
O=CC(CO)C(=O)O->O=CCC=O+O=CO
O=CO+OC#CCO->O=CC(C=O)C(=O)O
O=CC(C=O)C(=O)O->O=CC#CO+O=CO
O=CC#CO+O=CO->O=C=C(=C=O)C(=O)O
O=C=C(=C=O)C(=O)O->O=CCCCO+O=CO
OCCCCO->C#CO+C=O
C#CO+C=O->O=CCCCO
OCCCCO->C=O+CC=O
O=C=C(C=O)C(=O)O->O=CO+OC1CC1O
OC1CC1O+OCO->O=C=C(=C=O)C(=O)O
O=C=C(=C=O)C(=O)O->O=CO+OCCCCO