

Preparations

```
Quit[];
```

```
SetDirectory[NotebookDirectory[]];
```

```
Needs["ReactionKinetics1"]; // AbsoluteTiming
```

ReactionKinetics Version 1.0 [06-01-2013] using Mathematica
Version 8.0 for Microsoft Windows (32-bit) (November 7, 2010)
(Version 8., Release 0) loaded 30 April 2013 at 03:19 GMT+01:59
GNU General Public License (GPLv3) Terms Apply.

Please report reaction kinetics issues or problems at
nagyal@math.bme.hu, dpapp@iems.northwestern.edu, or jtoth@math.bme.hu

```
{0.4990285, Null}
```

Hydrogen combustion mechanisms

```
SetDirectory[NotebookDirectory[] <> "hydrogen"];
```

```
ClearAll[hdat, hdata];  
hdat = Flatten[Import["names_hydrogen.txt", "Table"]];  
hdata = StringReplace[#, ".dat" → ""] & /@ hdat  
  
{Ahmed2007, Burke2012, CRECK2012, Dagaut2003, Davis2005, GRI30, Hong2011,  
Keromnes2013, Konnov2008, Li2007, NUIG2010, OConaire2004, Rasmussen2008,  
SanDiego2011, SaxenaWilliams2006, Starik2009, Sun2007, USC2007, Zsely2005}
```

```
indices = Range[19];
```

```
TableForm[hdata, TableHeadings → {indices, None}]
```

```
1 | Ahmed2007
2 | Burke2012
3 | CRECK2012
4 | Dagaut2003
5 | Davis2005
6 | GRI30
7 | Hong2011
8 | Keromnes2013
9 | Konnov2008
10 | Li2007
11 | NUIG2010
12 | OConaire2004
13 | Rasmussen2008
14 | SanDiego2011
15 | SaxenaWilliams2006
16 | Starik2009
17 | Sun2007
18 | USC2007
19 | Zsely2005
```

```
ClearAll[hall];
hall = CHEMKINImport[#] ["chemkinreactions"] & /@ hdat; // AbsoluteTiming
```

```
{1.6380937, Null}
```

```
ClearAll[hevery];
hevery = Transpose[{hall, DeleteAutocatalysis /@ hall, hdata}]; //
AbsoluteTiming
```

```
{0.4320247, Null}
```

```
TableForm[
  ReactionsData[#, ExternalSpecies → {"HV"}] ["M", "R", "deficiency"] & /@
    hevery[[indices, 2]],
  TableHeadings → {hevery[[indices, 3]], {"M", "R", "deficiency"}}]
```

	M	R	deficiency
Ahmed2007	8	38	$\delta=n-l-s=29-11-6=12$
Burke2012	8	38	$\delta=n-l-s=31-12-6=13$
CRECK2012	8	37	$\delta=n-l-s=29-11-6=12$
Dagaut2003	8	42	$\delta=n-l-s=31-12-6=13$
Davis2005	8	40	$\delta=n-l-s=31-12-6=13$
GRI30	8	40	$\delta=n-l-s=31-12-6=13$
Hong2011	8	40	$\delta=n-l-s=31-12-6=13$
Keromnes2013	9	42	$\delta=n-l-s=32-12-7=13$
Konnov2008	8	42	$\delta=n-l-s=31-12-6=13$
Li2007	8	38	$\delta=n-l-s=31-12-6=13$
NUIG2010	8	38	$\delta=n-l-s=31-12-6=13$
OConaire2004	8	38	$\delta=n-l-s=31-12-6=13$
Rasmussen2008	8	40	$\delta=n-l-s=31-12-6=13$
SanDiego2011	8	42	$\delta=n-l-s=31-12-6=13$
SaxenaWilliams2006	8	42	$\delta=n-l-s=31-12-6=13$
Starik2009	9	52	$\delta=n-l-s=41-16-7=18$
Sun2007	8	40	$\delta=n-l-s=31-12-6=13$
USC2007	8	40	$\delta=n-l-s=31-12-6=13$
Zsely2005	8	42	$\delta=n-l-s=31-12-6=13$

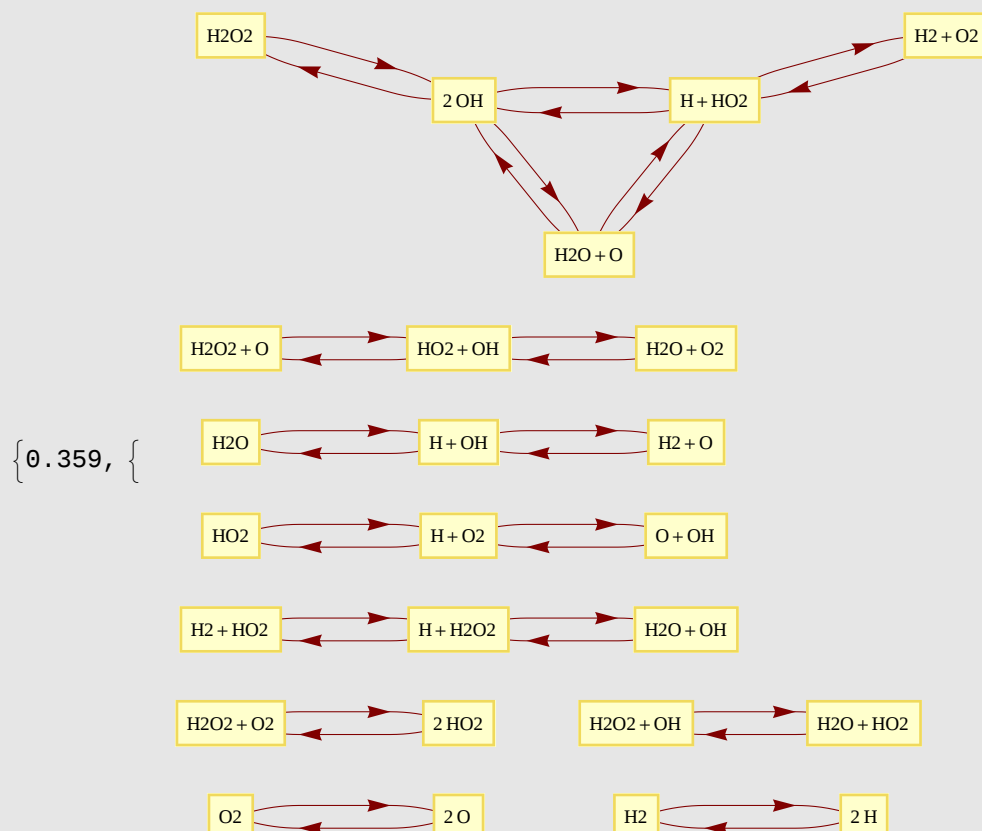
```
TableForm[
  ReactionsData[#, ExternalSpecies → "HV"] ["species"] & /@ hevery[[indices, 2]],
  TableHeadings → {hevery[[indices, 3]], {"list", " of ", "species\n"}}]
```

	list	of	species					
Ahmed2007	H	H2	H2O	OH	H2O2	H02	O2	0
Burke2012	H	H2	H2O	OH	H2O2	H02	O2	0
CRECK2012	H2O2	0	H02	OH	H	H2	H2O	O2
Dagaut2003	H	H2	H2O	OH	H2O2	H02	O2	0
Davis2005	H	H2	H2O	OH	H2O2	H02	O2	0
GRI30	H	H2	H2O	OH	H2O2	H02	O2	0
Hong2011	H	H2	H2O	OH	H2O2	H02	O2	0
Keromnes2013	H	H2	H2O	OH	H2O2	H02	O2	0
Konnov2008	H	H2	H2O	OH	H2O2	H02	O2	0
Li2007	H	H2	H2O	OH	H2O2	H02	O2	0
NUIG2010	H	H2	H2O	OH	H2O2	H02	O2	0
OConaire2004	H	H2	H2O	OH	H2O2	H02	O2	0
Rasmussen2008	H	H2	H2O	OH	H2O2	H02	O2	0
SanDiego2011	H	H2	H2O	OH	H2O2	H02	O2	0
SaxenaWilliams2006	H	H2	H2O	OH	H2O2	H02	O2	0
Starik2009	H	H2	H2O	OH	H2O2	H02	O2	0
Sun2007	H	H2	H2O	OH	H2O2	H02	O2	0
USC2007	H	H2	H2O	OH	H2O2	H02	O2	0
Zsely2005	H	H2	H2O	OH	H2O2	H02	O2	0

Ahmed2007
Burke2012
CRECK2012
Dagaut2003
Davis2005
GRI30
Hong2011
Keromnes2013
Konnov2008
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OConaire2004
Rasmussen2008
SanDiego2011
SaxenaWilliams2006
Starik2009
Sun2007
USC2007
Zsely2005

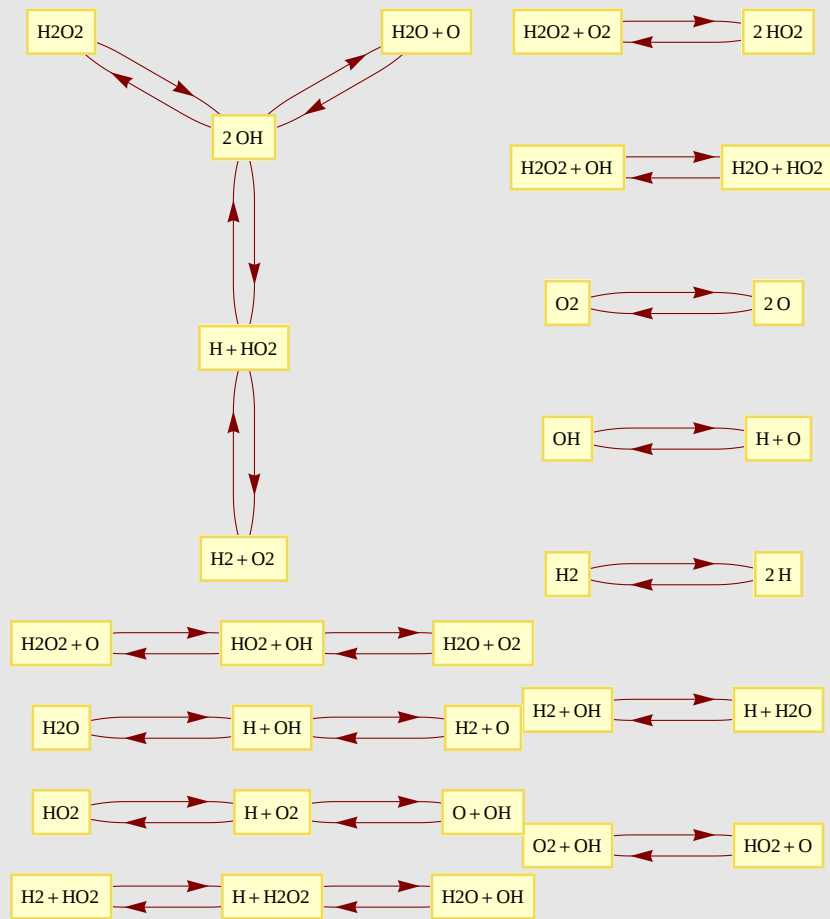
$$\{ \text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O} + \text{OH} \}$$

Ahmed2007

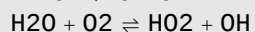
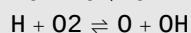
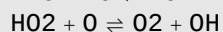
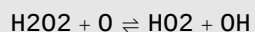
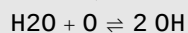
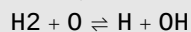
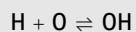
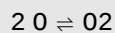
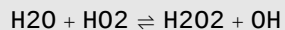
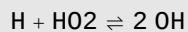
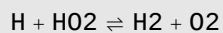
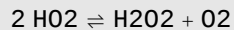
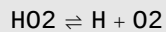
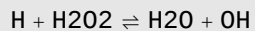
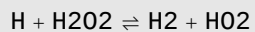
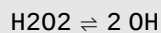
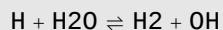
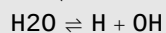
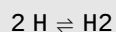


3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{HO}_2 \rightleftharpoons 2\text{OH}$
$\text{HO}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$2\text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H} + \text{HO}_2 \rightleftharpoons 2\text{OH}$	$2\text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$
$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$2\text{H} \rightleftharpoons \text{H}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{HO}_2 + \text{OH}$	$2\text{O} \rightleftharpoons \text{O}_2$

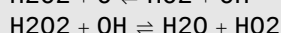
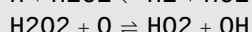
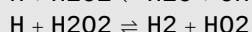
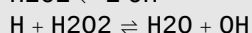
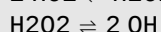
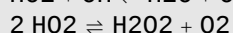
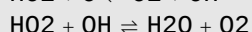
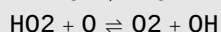
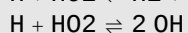
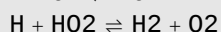
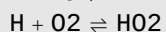
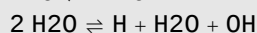
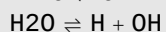
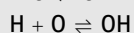
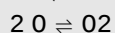
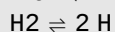
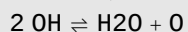
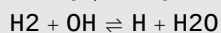
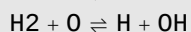
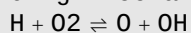
Burke2012



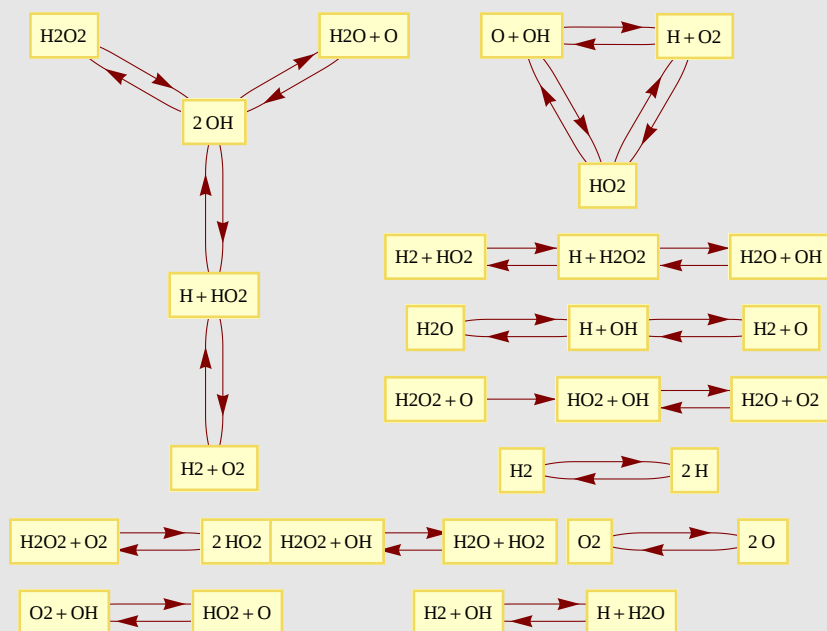
3rd body species deleted



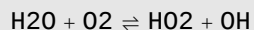
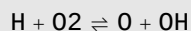
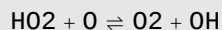
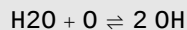
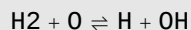
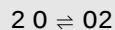
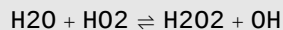
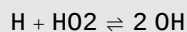
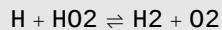
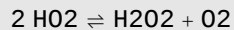
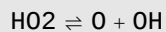
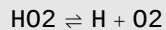
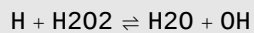
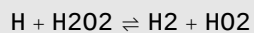
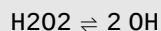
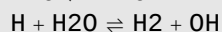
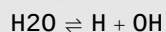
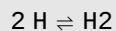
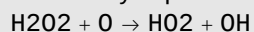
Orig. Mechanism



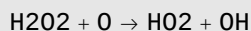
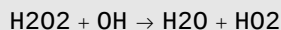
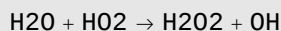
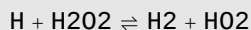
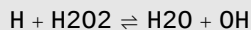
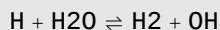
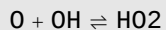
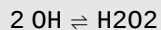
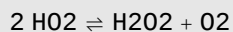
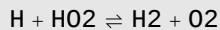
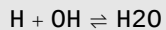
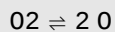
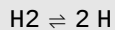
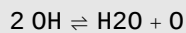
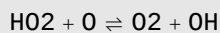
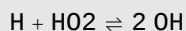
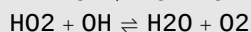
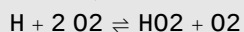
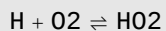
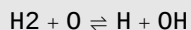
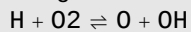
CRECK2012



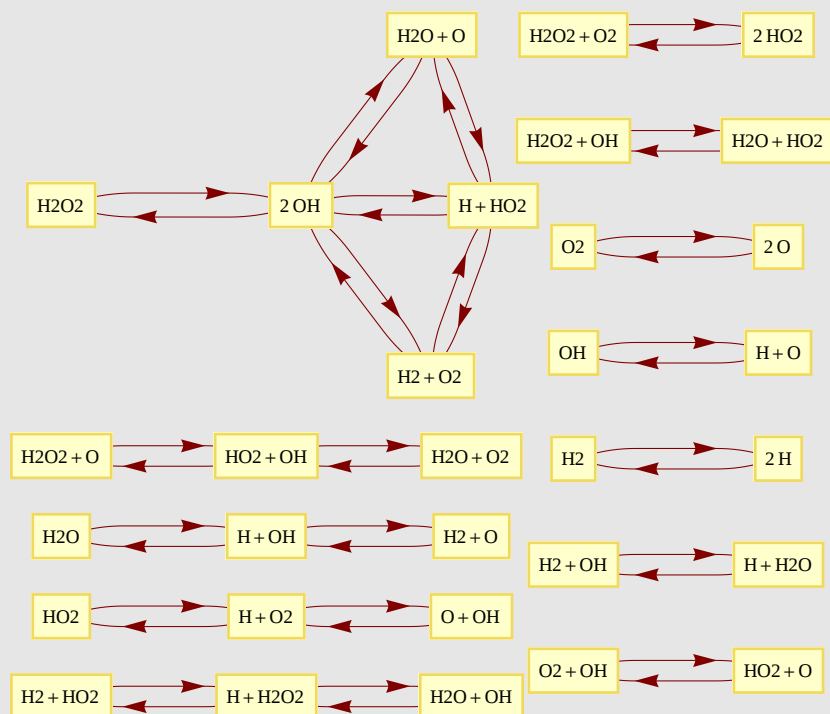
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Orig. Mechanism

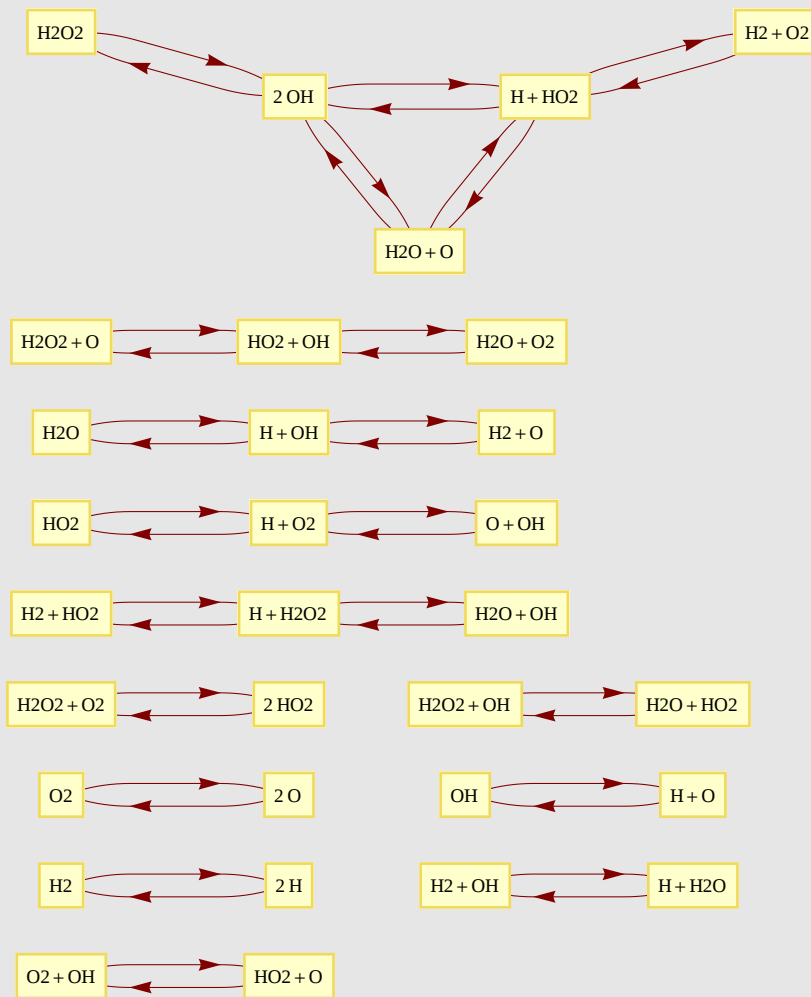


Dagaut2003



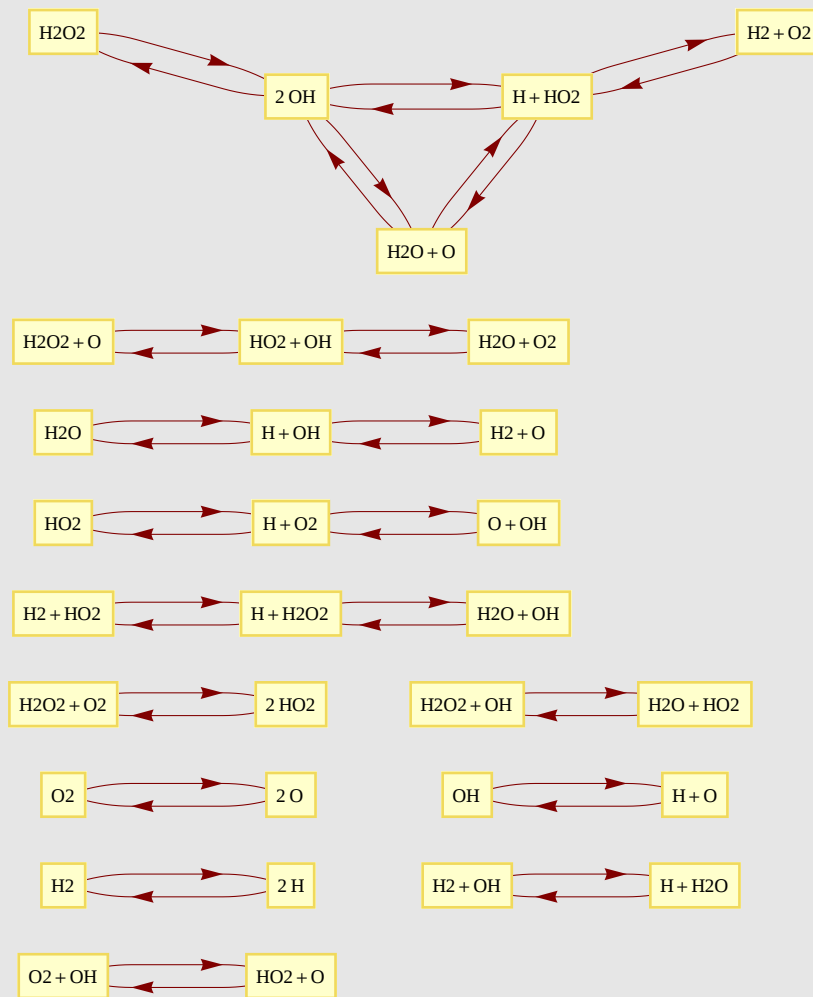
3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$2\text{H} \rightleftharpoons \text{H}_2$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$2\text{O} \rightleftharpoons \text{O}_2$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}_2$
$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$

Davis2005

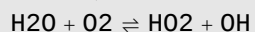
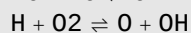
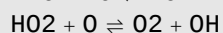
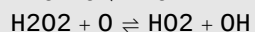
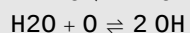
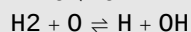
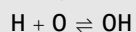
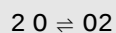
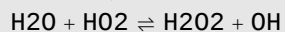
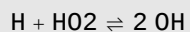
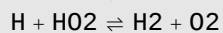
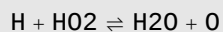
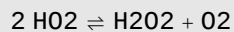
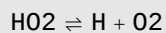
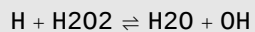
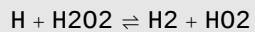
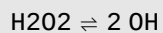
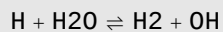
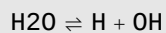
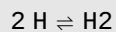


3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$2\text{H} \rightleftharpoons \text{H}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$2\text{H} + \text{H}_2 \rightleftharpoons 2\text{H}_2$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{O}_2$	$2\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$
$2\text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{O}_2$	$2\text{O} \rightleftharpoons \text{O}_2$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons 2\text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}_2$
$2\text{O} \rightleftharpoons \text{O}_2$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O} \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$2\text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
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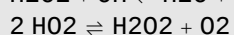
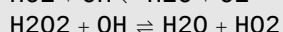
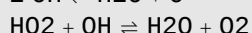
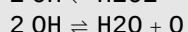
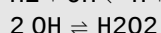
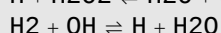
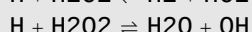
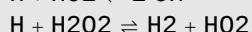
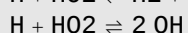
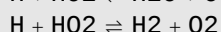
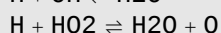
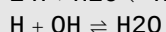
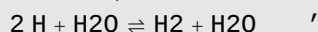
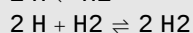
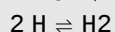
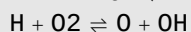
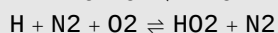
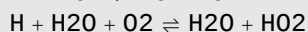
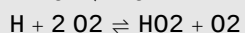
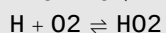
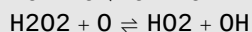
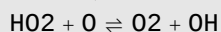
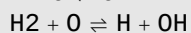
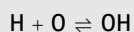
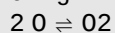
GRI30



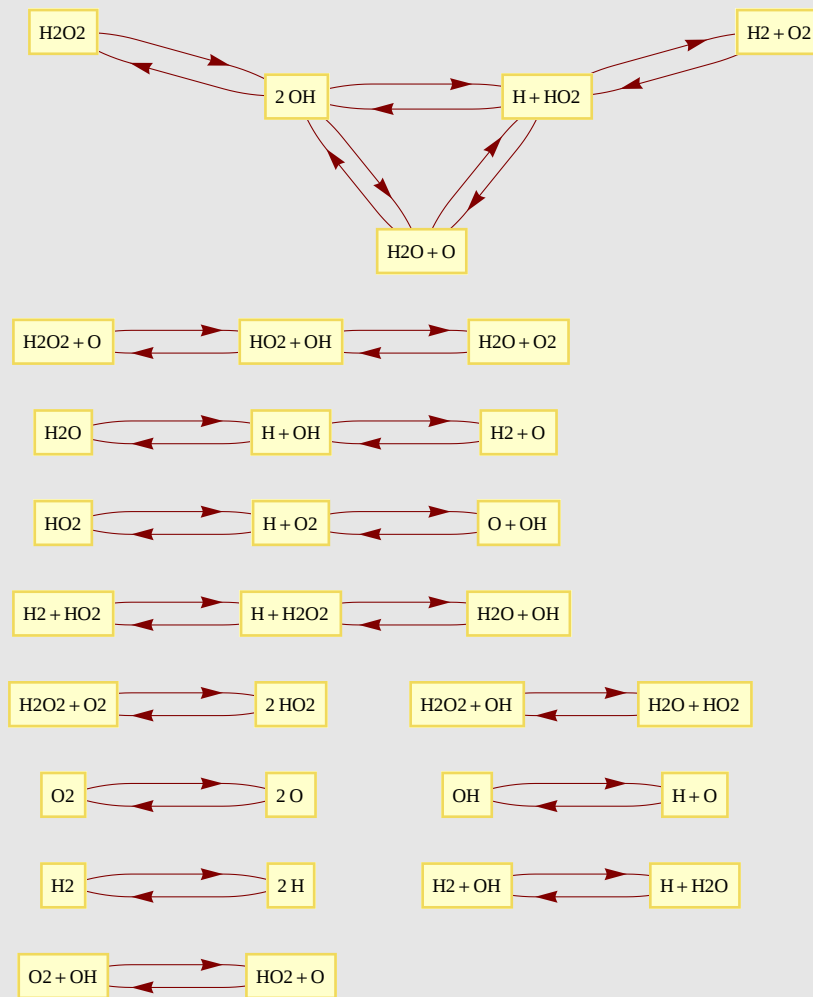
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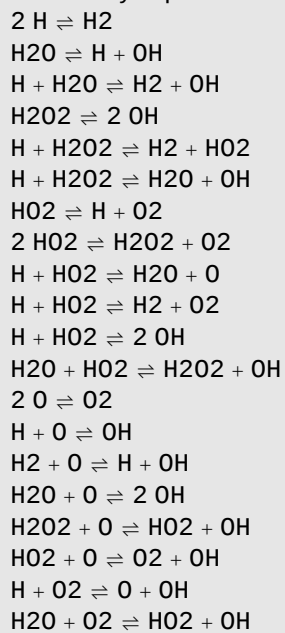
Orig. Mechanism



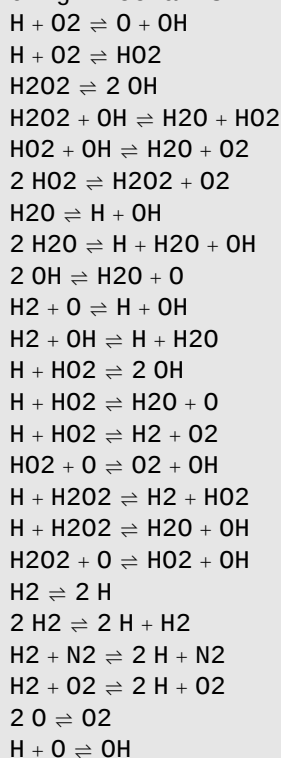
Hong2011



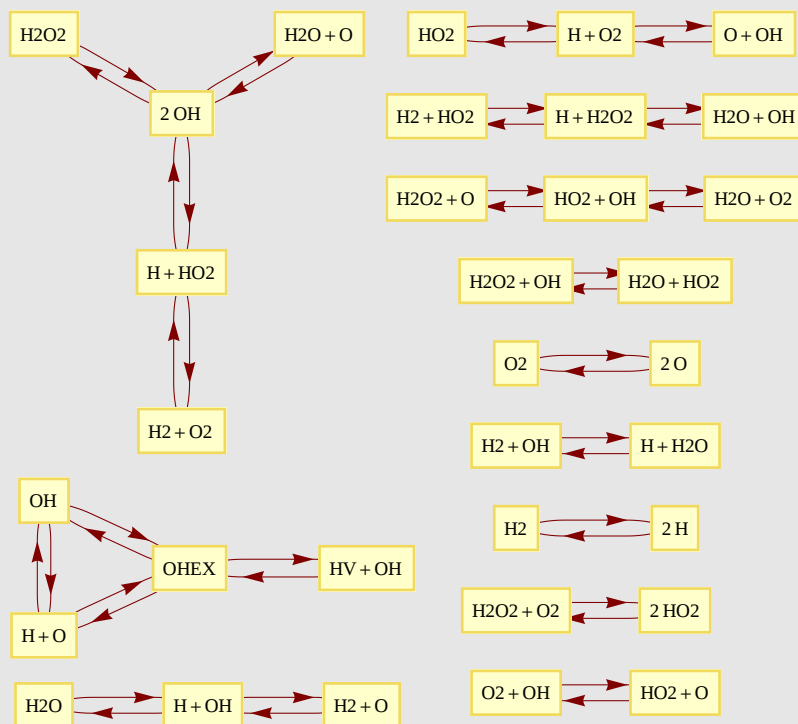
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Orig. Mechanism

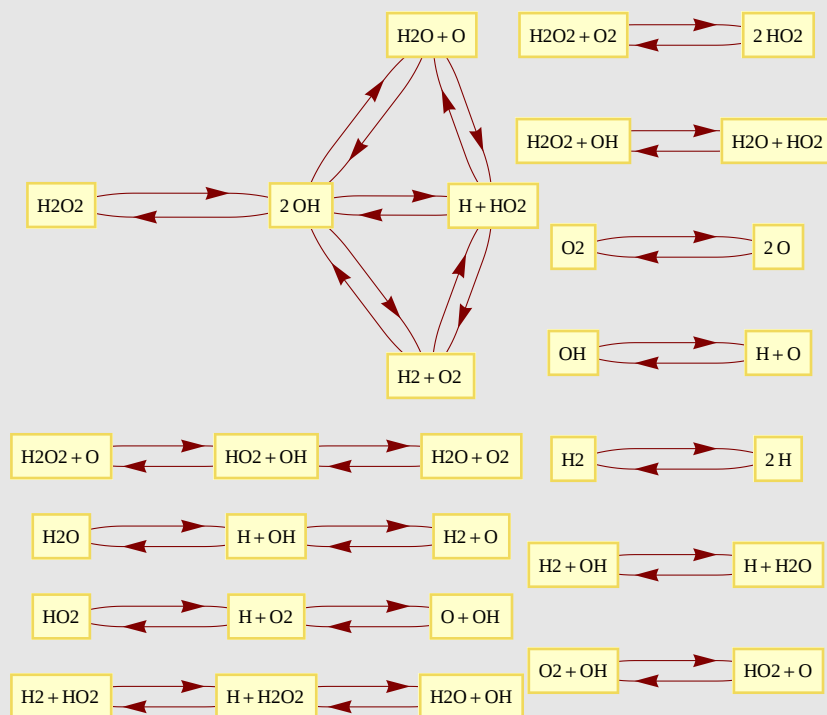


Keromnes2013

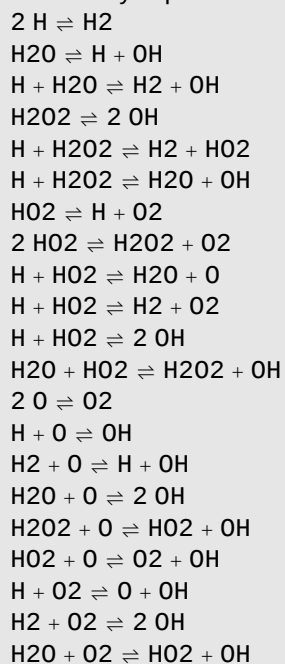


	Orig. Mechanism
3rd body species deleted	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$2 \text{H} \rightleftharpoons \text{H}_2$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2 \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$	$\text{H}_2 \rightleftharpoons 2 \text{H}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$2 \text{O} \rightleftharpoons \text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$2 \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$	$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$2 \text{O} \rightleftharpoons \text{O}_2$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$2 \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$,
$\text{H} + \text{O} \rightleftharpoons \text{OHEX}$	$\text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2 \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{O} \rightleftharpoons \text{OHEX}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O} + \text{OHEX} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{OH} \rightleftharpoons \text{OHEX}$	$\text{H}_2 + \text{OHEX} \rightleftharpoons \text{H}_2 + \text{OH}$
$\text{HV} + \text{OH} \rightleftharpoons \text{OHEX}$	$\text{N}_2 + \text{OHEX} \rightleftharpoons \text{N}_2 + \text{OH}$
	$\text{OH} + \text{OHEX} \rightleftharpoons 2 \text{OH}$
	$\text{H} + \text{OHEX} \rightleftharpoons \text{H} + \text{OH}$
	$\text{OHEX} \rightleftharpoons \text{OH}$
	$\text{OHEX} \rightleftharpoons \text{HV} + \text{OH}$
	$\text{O}_2 + \text{OHEX} \rightleftharpoons \text{O}_2 + \text{OH}$

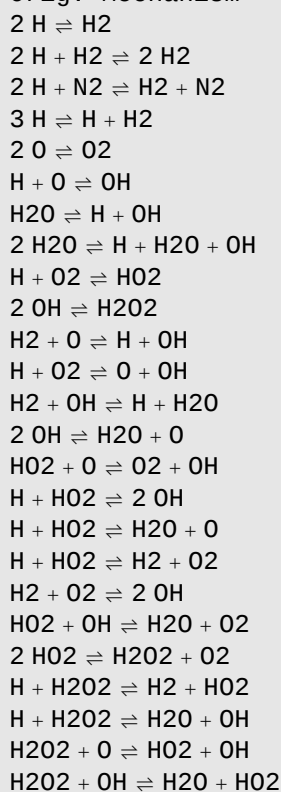
Konnov2008



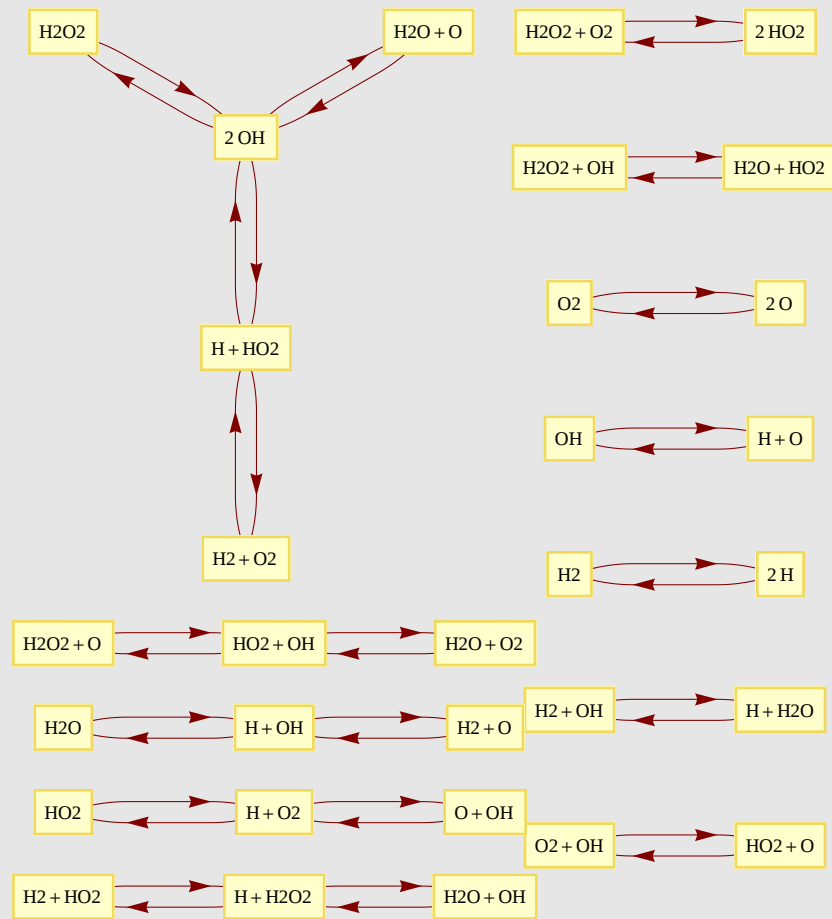
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Orig. Mechanism

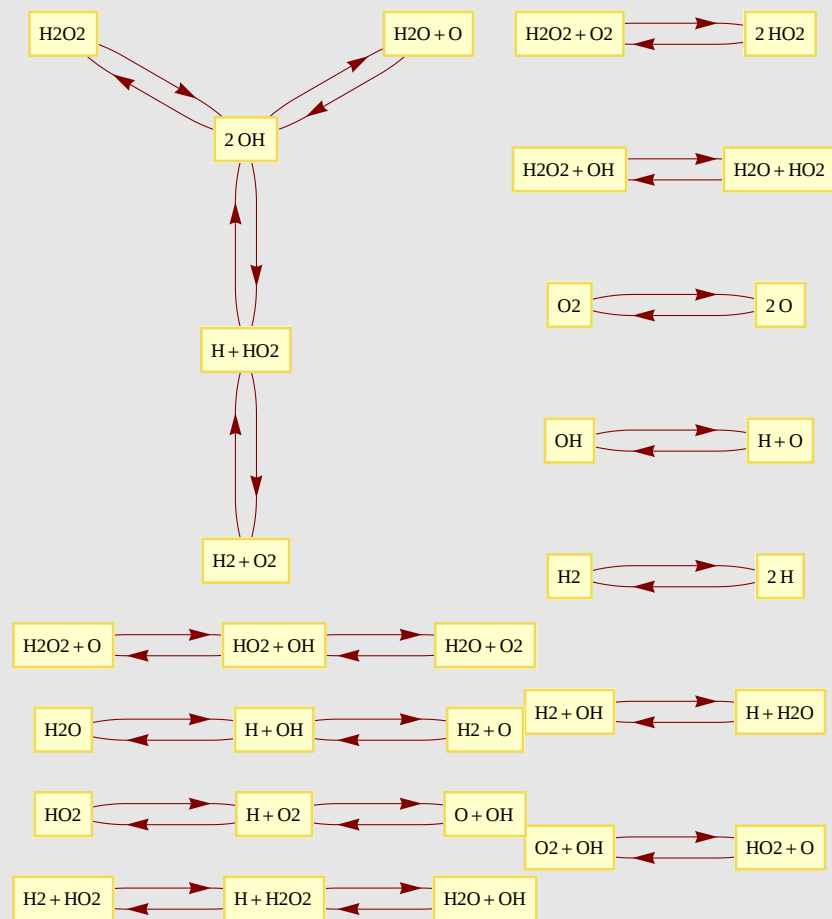


Li2007



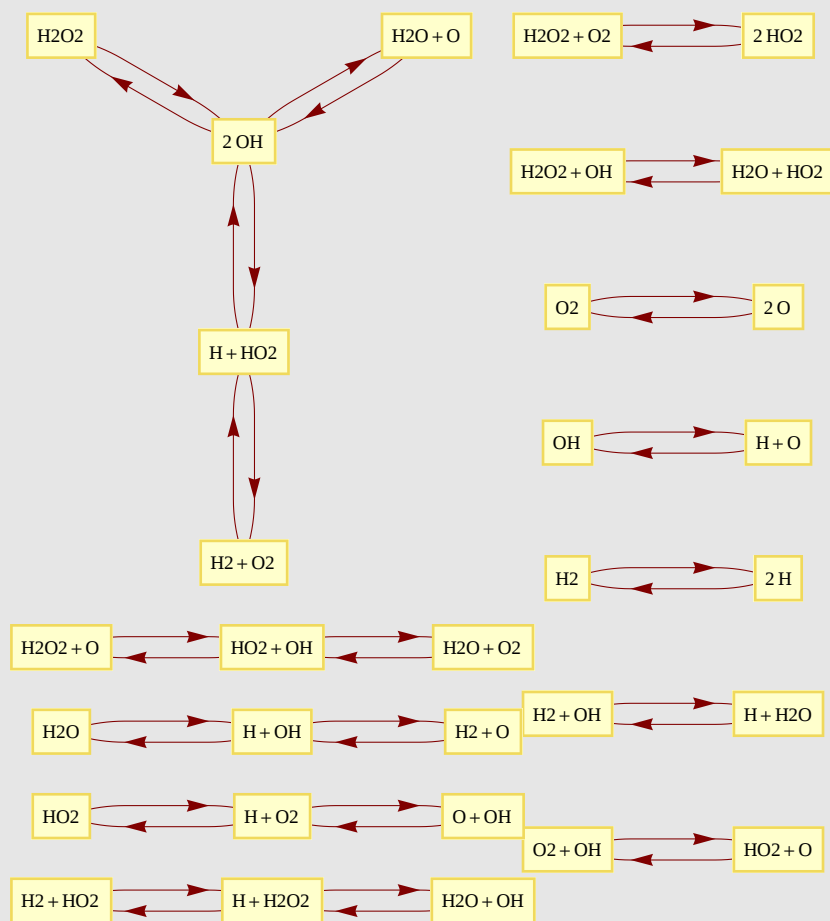
3rd body species deleted	Orig. Mechanism
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$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$\text{H}_2 \rightleftharpoons 2\text{H}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$2\text{O} \rightleftharpoons \text{O}_2$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$

NUIG2010



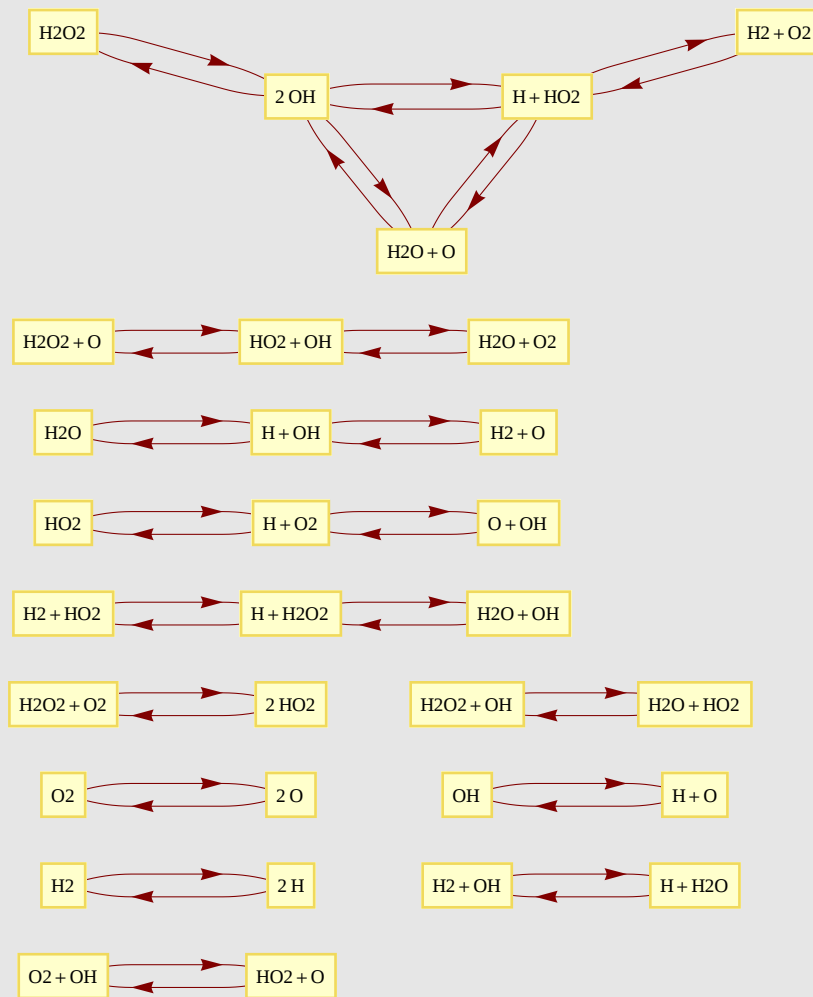
3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$\text{H}_2 \rightleftharpoons 2\text{H}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{O}_2 \rightleftharpoons 2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{OH} \rightleftharpoons \text{H} + \text{O}$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O}_2 \rightleftharpoons 2\text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$

OConaire2004

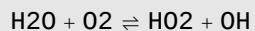
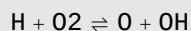
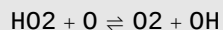
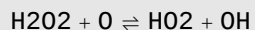
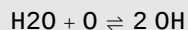
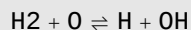
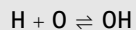
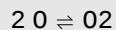
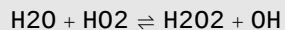
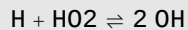
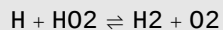
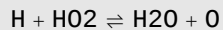
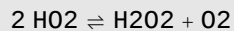
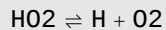
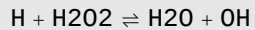
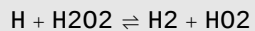
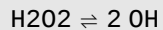
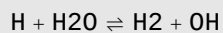
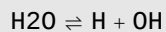
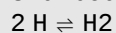


3rd body species deleted	Orig. Mechanism
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$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$\text{H}_2 \rightleftharpoons 2\text{H}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{O}_2 \rightleftharpoons 2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{OH} \rightleftharpoons \text{H} + \text{O}$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O}_2 \rightleftharpoons 2\text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$

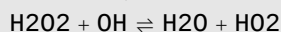
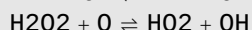
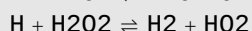
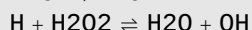
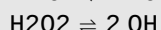
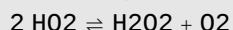
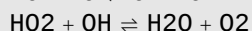
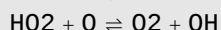
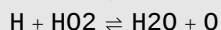
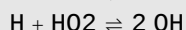
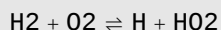
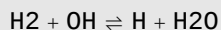
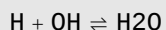
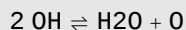
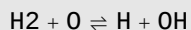
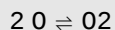
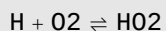
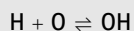
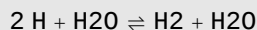
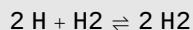
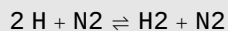
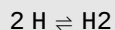
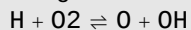
Rasmussen2008



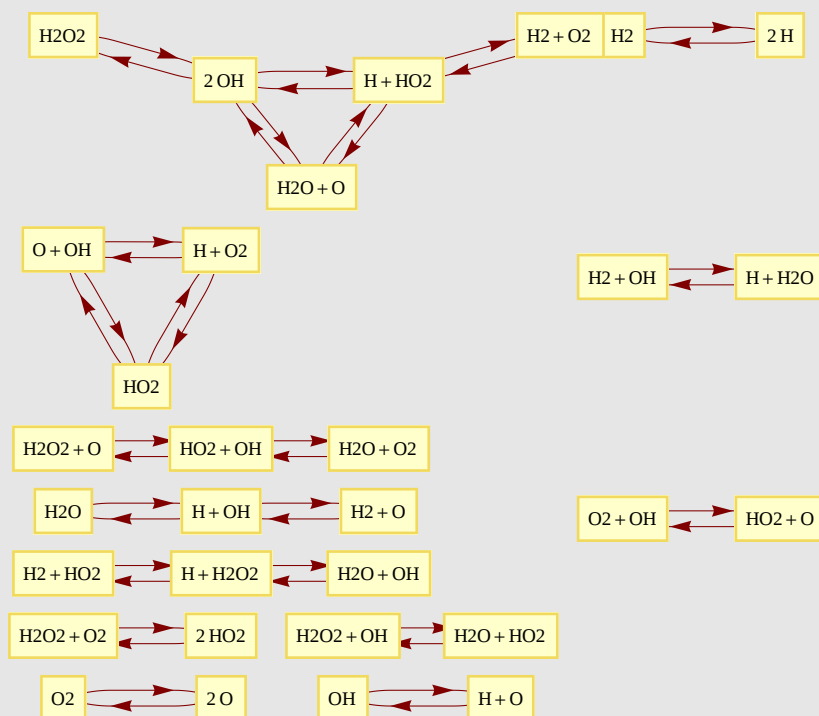
3rd body species deleted



Orig. Mechanism

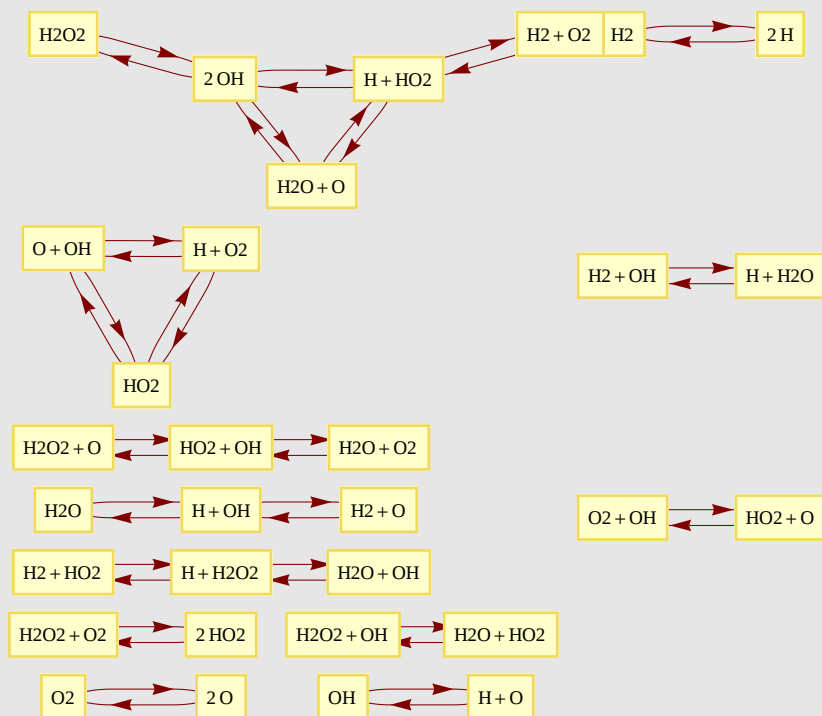


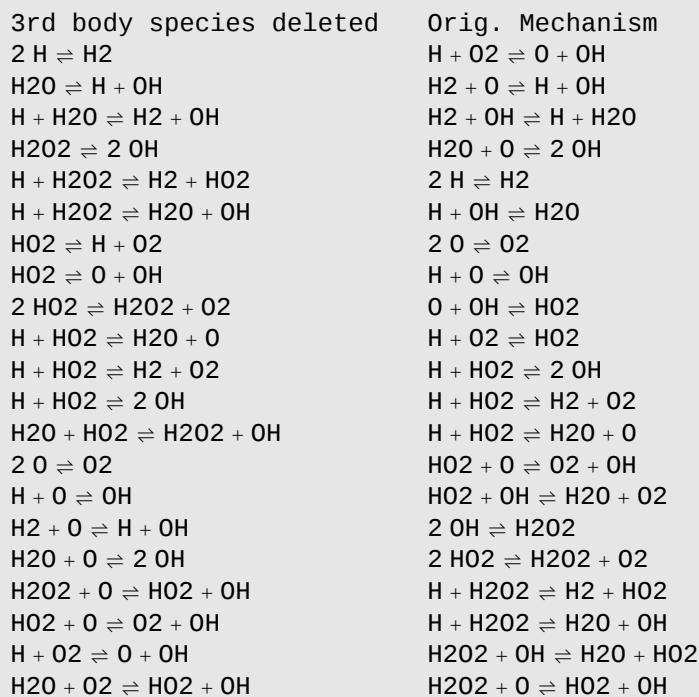
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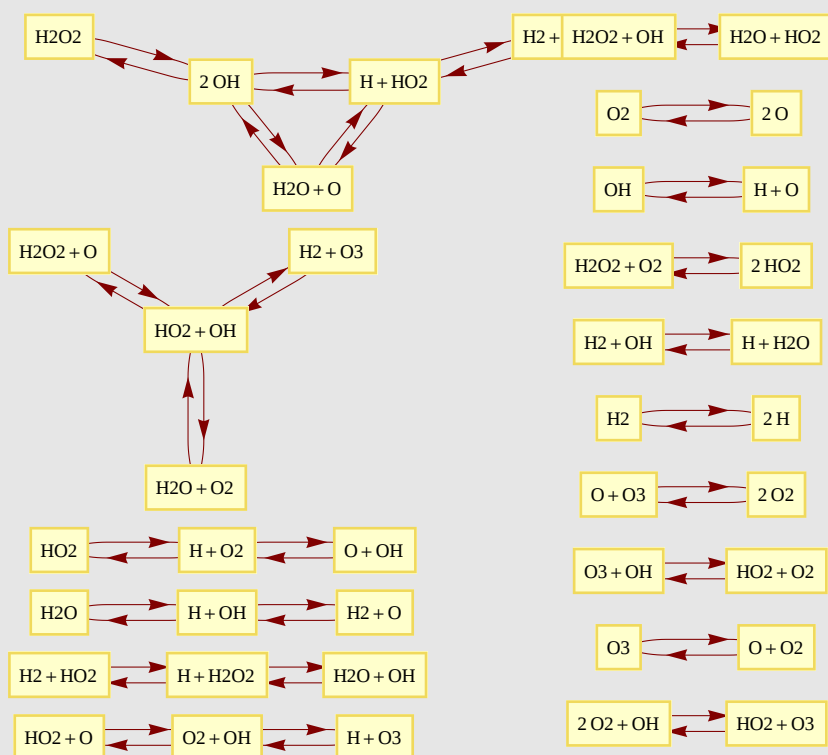
3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$	$2\text{H} \rightleftharpoons \text{H}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{HO}_2 \rightleftharpoons \text{H} + \text{O}_2$	$2\text{O} \rightleftharpoons \text{O}_2$
$\text{HO}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$2\text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{O} + \text{OH} \rightleftharpoons \text{HO}_2$
$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2$
$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H} + \text{HO}_2 \rightleftharpoons 2\text{OH}$
$\text{H} + \text{HO}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$2\text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$
$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{HO}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$

SaxenaWilliams2006



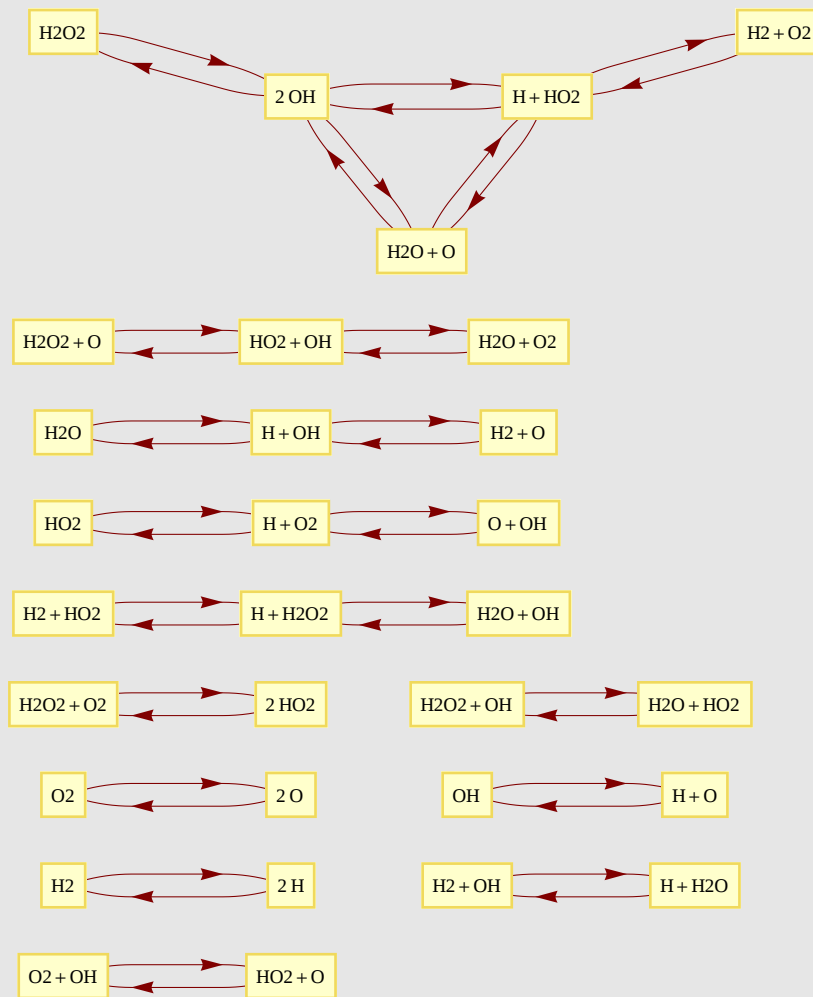


Starik2009

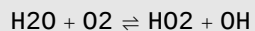
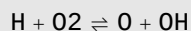
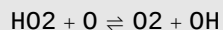
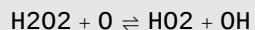
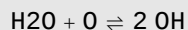
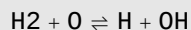
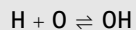
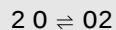
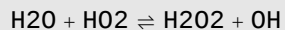
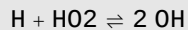
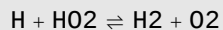
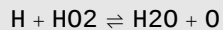
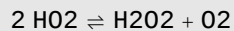
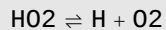
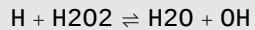
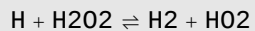
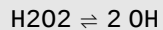
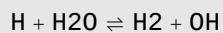
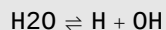
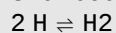


3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{O}_2 \rightleftharpoons 2\text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}$	$\text{H}_2 \rightleftharpoons 2\text{H}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{OH} \rightleftharpoons \text{H} + \text{O}$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons \text{H} + \text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$2\text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}_2$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$
$2\text{O}_2 \rightleftharpoons \text{O} + \text{O}_3$	$\text{H}_2\text{O}_2 + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O}_2 + \text{O}_2 \rightleftharpoons \text{O}_3 + \text{OH}$	$\text{O}_3 \rightleftharpoons \text{O} + \text{O}_2$
$\text{O} + \text{O}_2 \rightleftharpoons \text{O}_3$	$\text{H} + \text{O}_3 \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O}_3 \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{O} + \text{O}_3 \rightleftharpoons 2\text{O}_2$
$\text{H}_2 + \text{O}_3 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{O}_3 + \text{OH} \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O}_3 \rightleftharpoons 2\text{O}_2 + \text{OH}$	$\text{H}_2 + \text{O}_3 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$
	$\text{H}_2\text{O}_2 + \text{O}_3 \rightleftharpoons 2\text{O}_2 + \text{OH}$

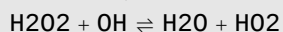
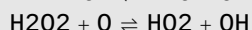
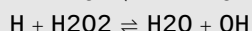
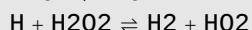
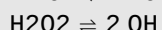
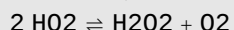
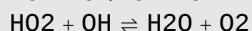
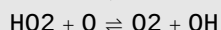
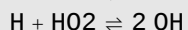
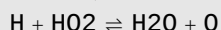
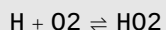
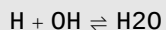
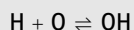
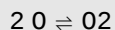
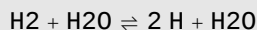
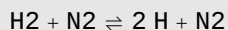
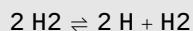
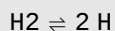
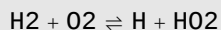
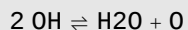
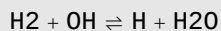
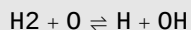
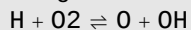
Sun2007



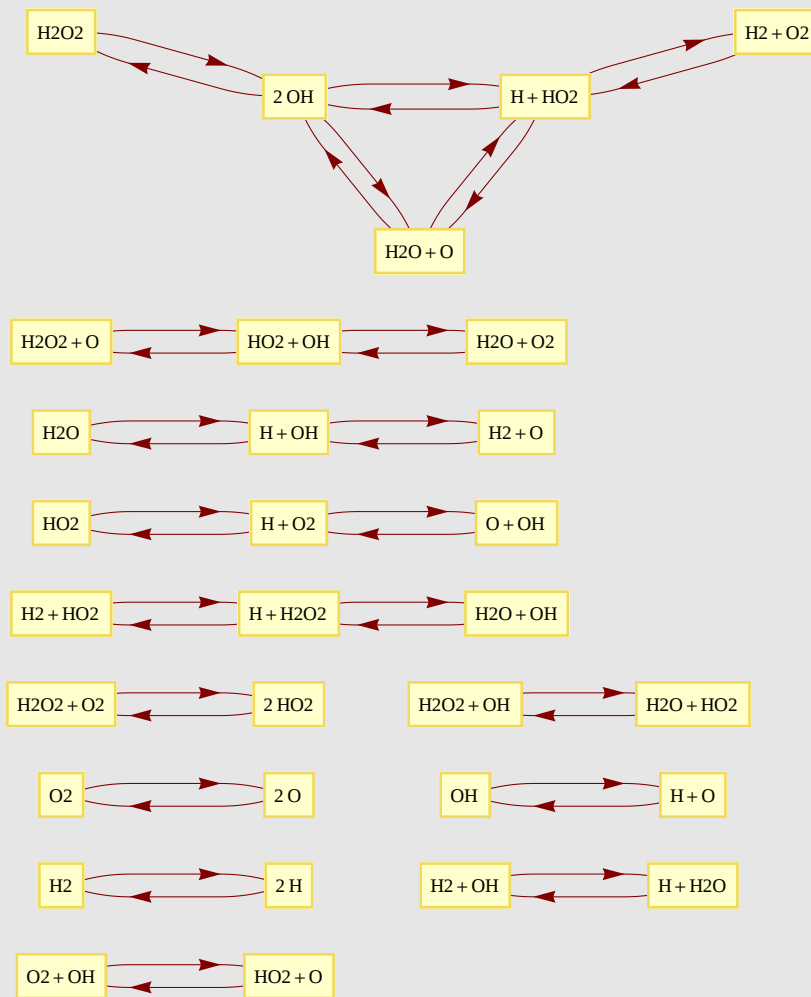
3rd body species deleted



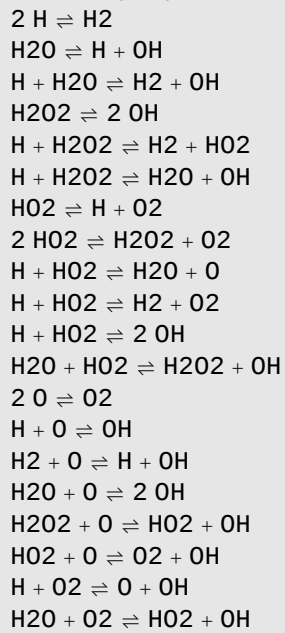
Orig. Mechanism



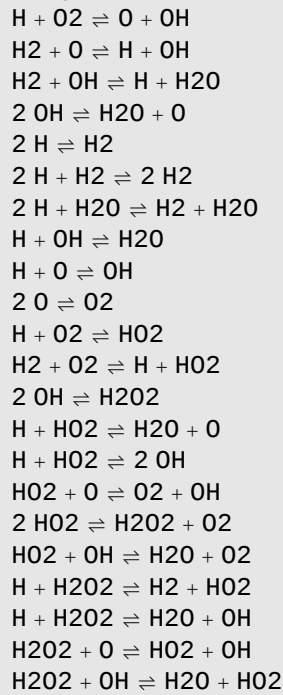
USC2007



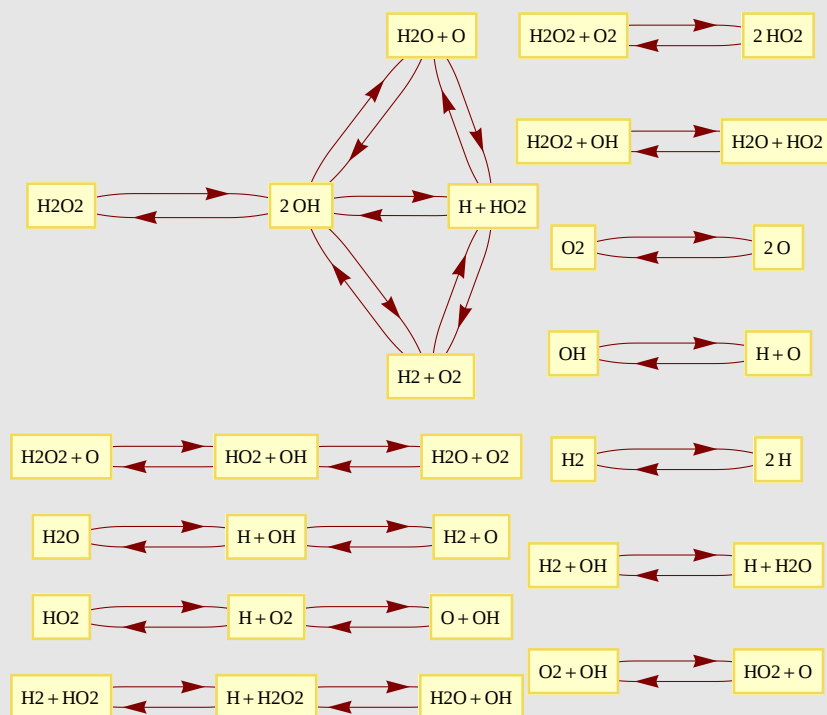
3rd body species deleted



Orig. Mechanism



Zsely2005



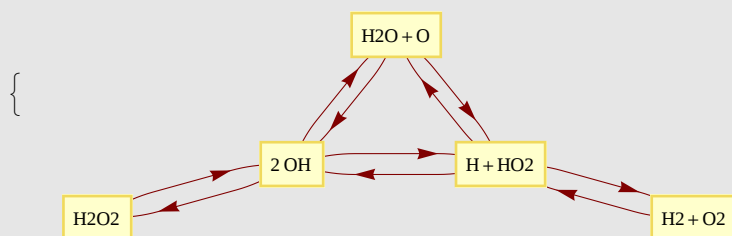
3rd body species deleted	Orig. Mechanism
$2\text{H} \rightleftharpoons \text{H}_2$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons \text{H} + \text{O}_2$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$	$2\text{H} \rightleftharpoons \text{H}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$	$2\text{H} + \text{H}_2 \rightleftharpoons 2\text{H}_2$ }}
$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$2\text{O} \rightleftharpoons \text{O}_2$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons 2\text{OH}$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2\text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$2\text{O} \rightleftharpoons \text{O}_2$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$2\text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$2\text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
	$\text{H}_2 + \text{O}_2 \rightleftharpoons 2\text{OH}$

```
maxfhjcomponents = MaxFHJWeaklyConnectedComponents[hevery[[#, 2]] & /@ indices;
```

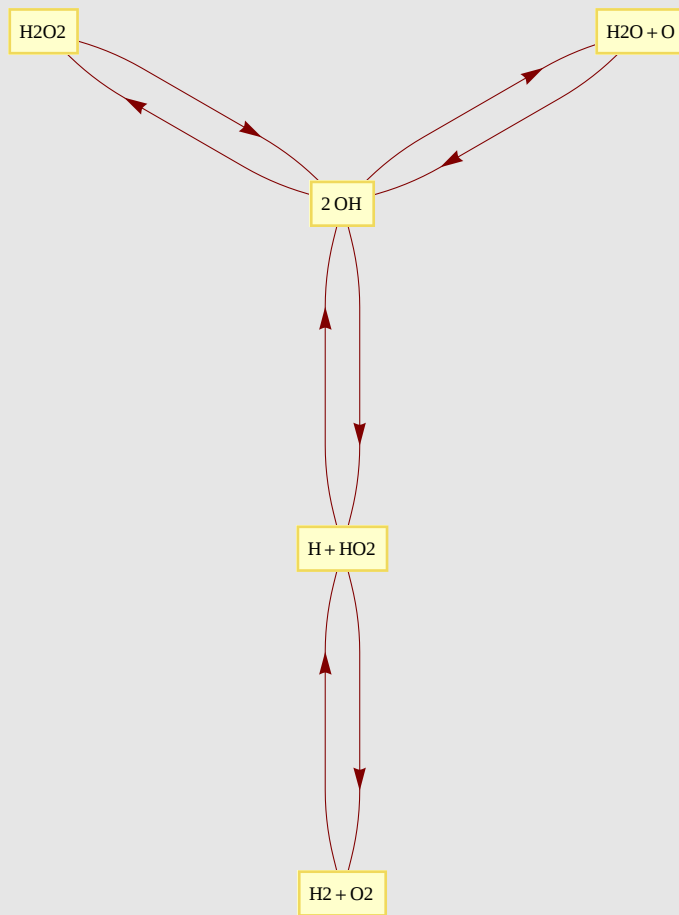
```
maxfhjedges = Flatten[(First /@ #) & /@ maxfhjcomponents, 1];
```

```
GraphPlot[First[#], VertexLabeling -> True, DirectedEdges -> True,
  ImageSize -> 350, PlotLabel -> "Max weakly connected component of mech "<>
  ToString[hevery[[Last[#], 3]] <> "\n"] & /@
  Transpose[{maxfhjedges, indices}]
```

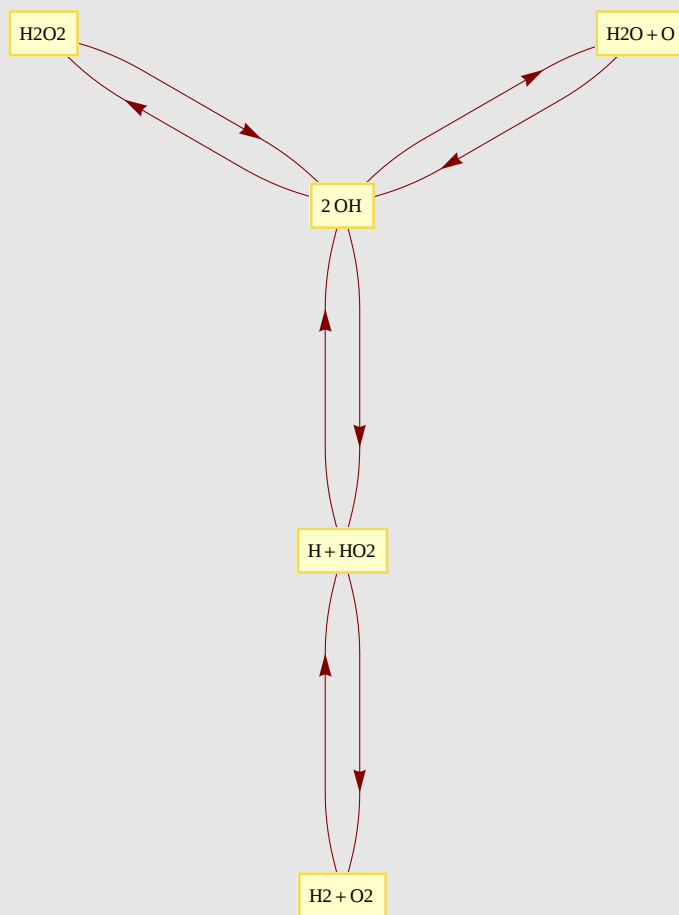
Max weakly connected component of mech Ahmed2007



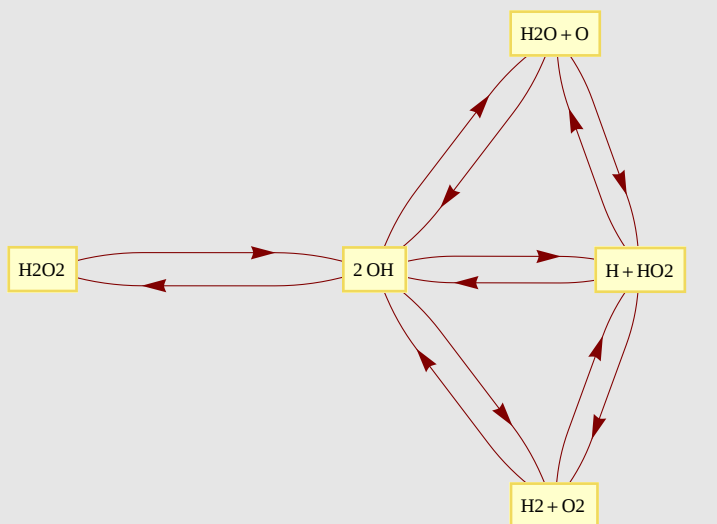
Max weakly connected component of mech Burke2012



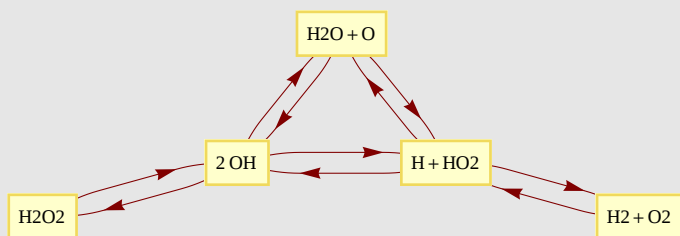
Max weakly connected component of mech CRECK2012



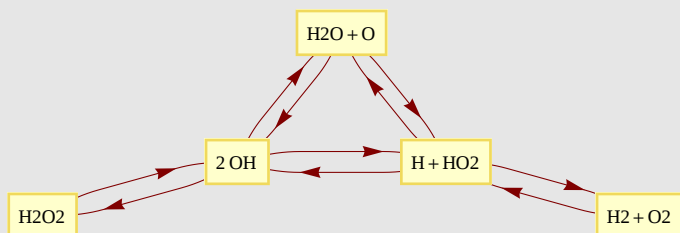
Max weakly connected component of mech Dagaut2003



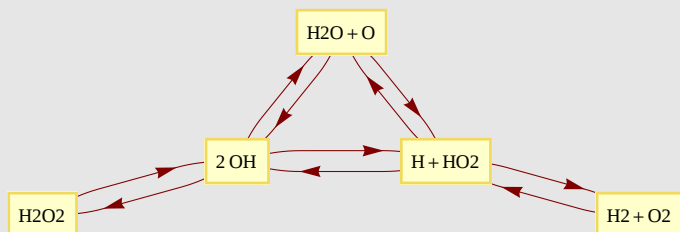
Max weakly connected component of mech Davis2005



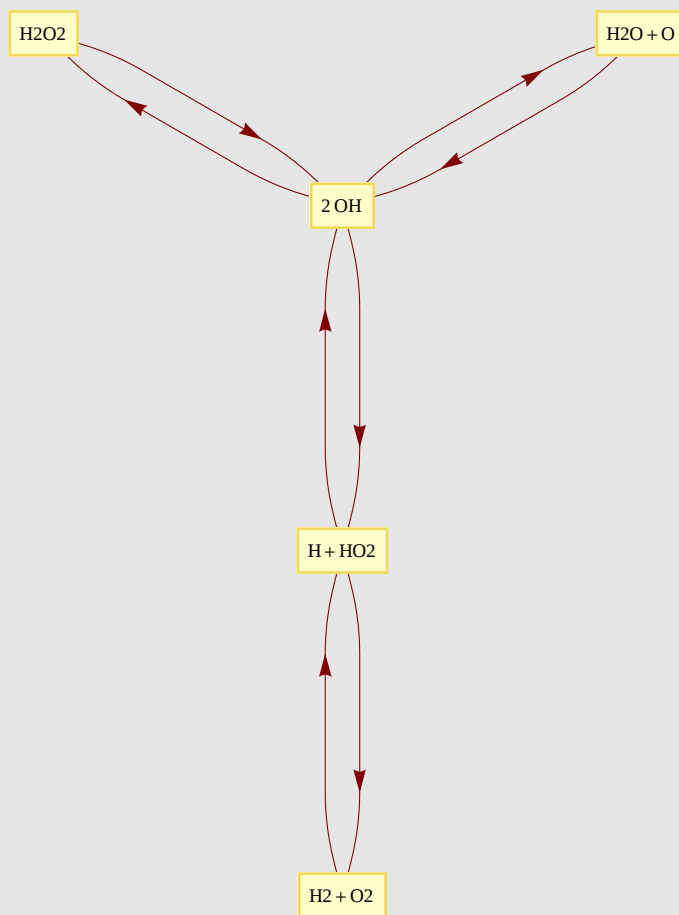
Max weakly connected component of mech GRI30



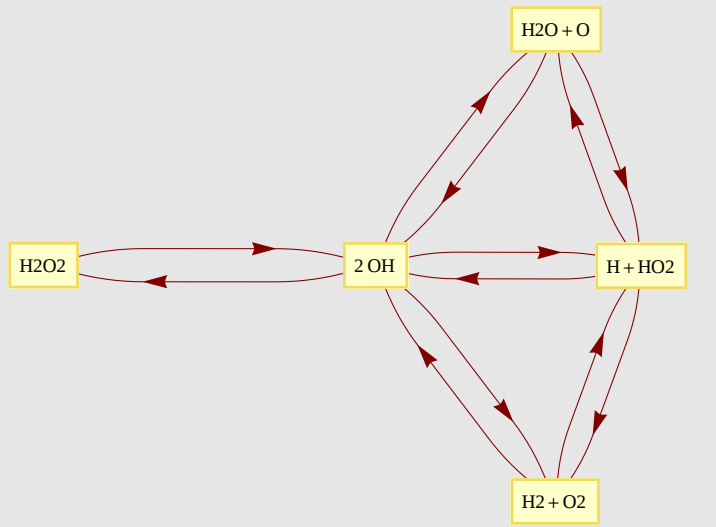
Max weakly connected component of mech Hong2011



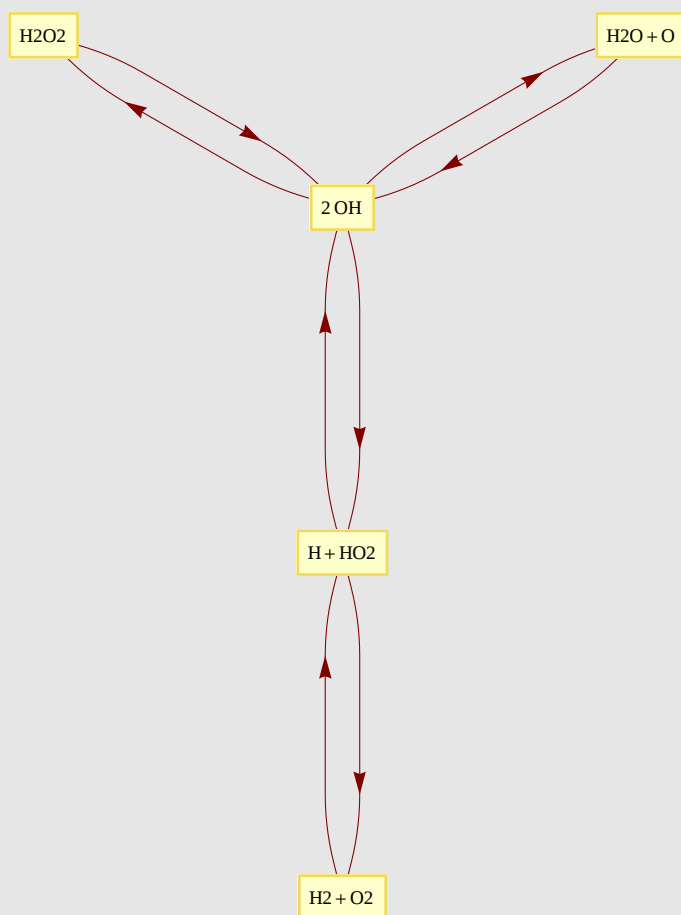
Max weakly connected component of mech Keromnes2013



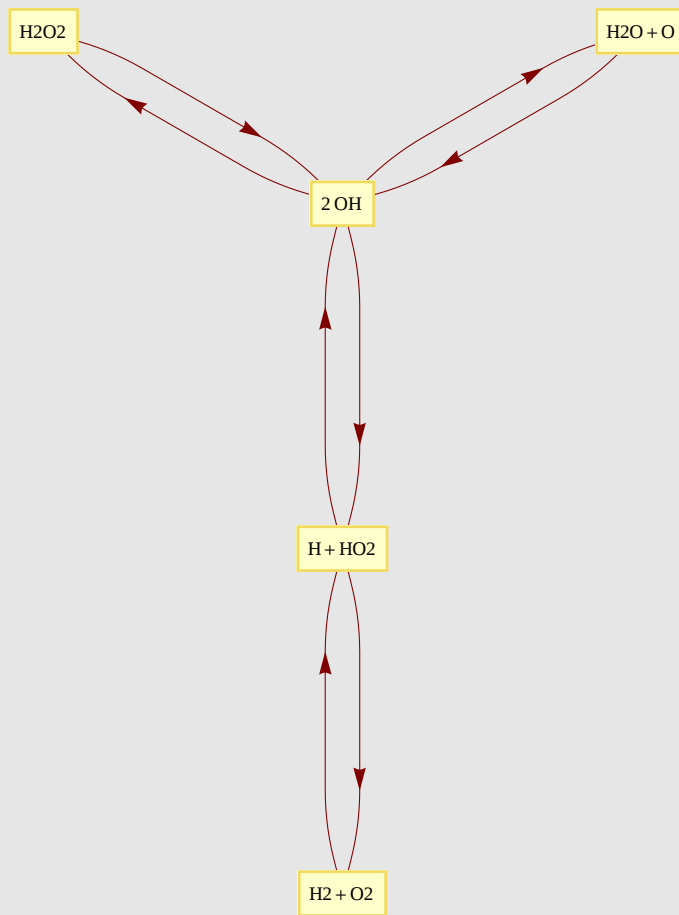
Max weakly connected component of mech Konnov2008



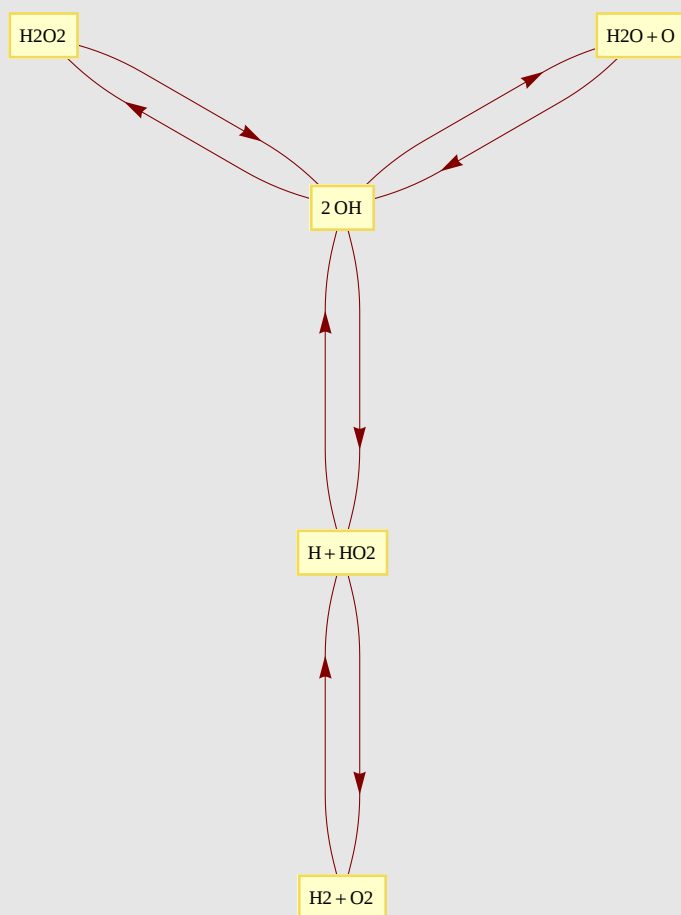
Max weakly connected component of mech Li2007



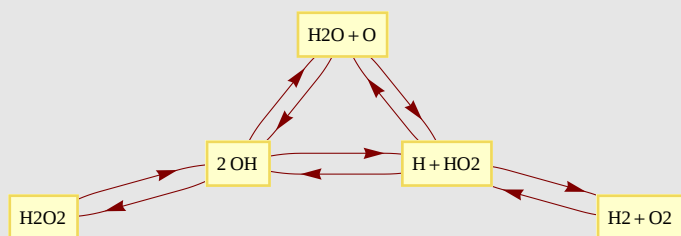
Max weakly connected component of mech NUIG2010



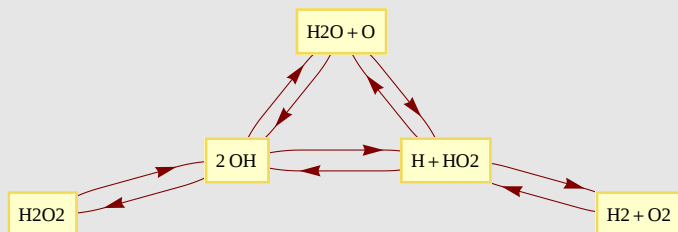
Max weakly connected component of mech OConaire2004



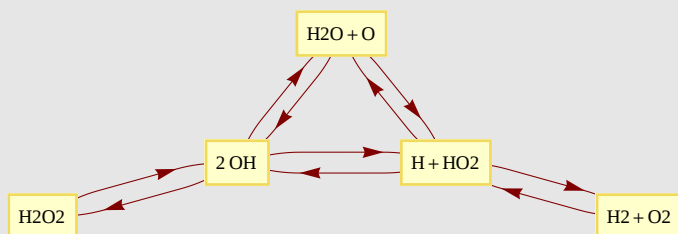
Max weakly connected component of mech Rasmussen2008



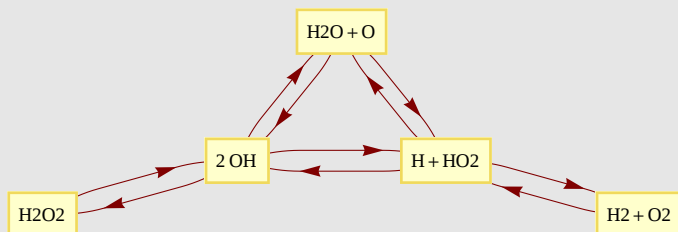
Max weakly connected component of mech SanDiego2011



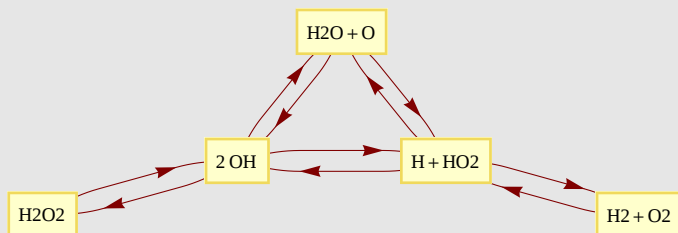
Max weakly connected component of mech SaxenaWilliams2006



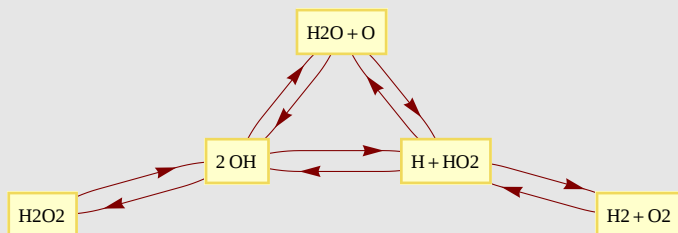
Max weakly connected component of mech Starik2009



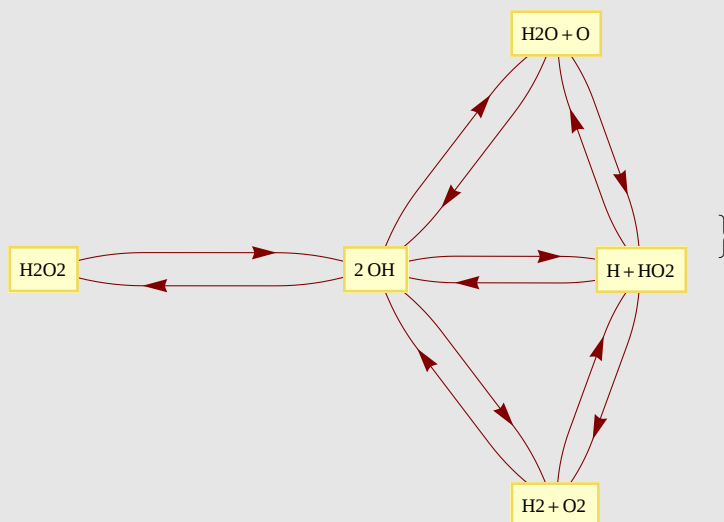
Max weakly connected component of mech Sun2007



Max weakly connected component of mech USC2007



Max weakly connected component of mech Zsely2005



```

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    {True -> Style["TRUE", Bold]}, {i, 19}, {j, 19}],
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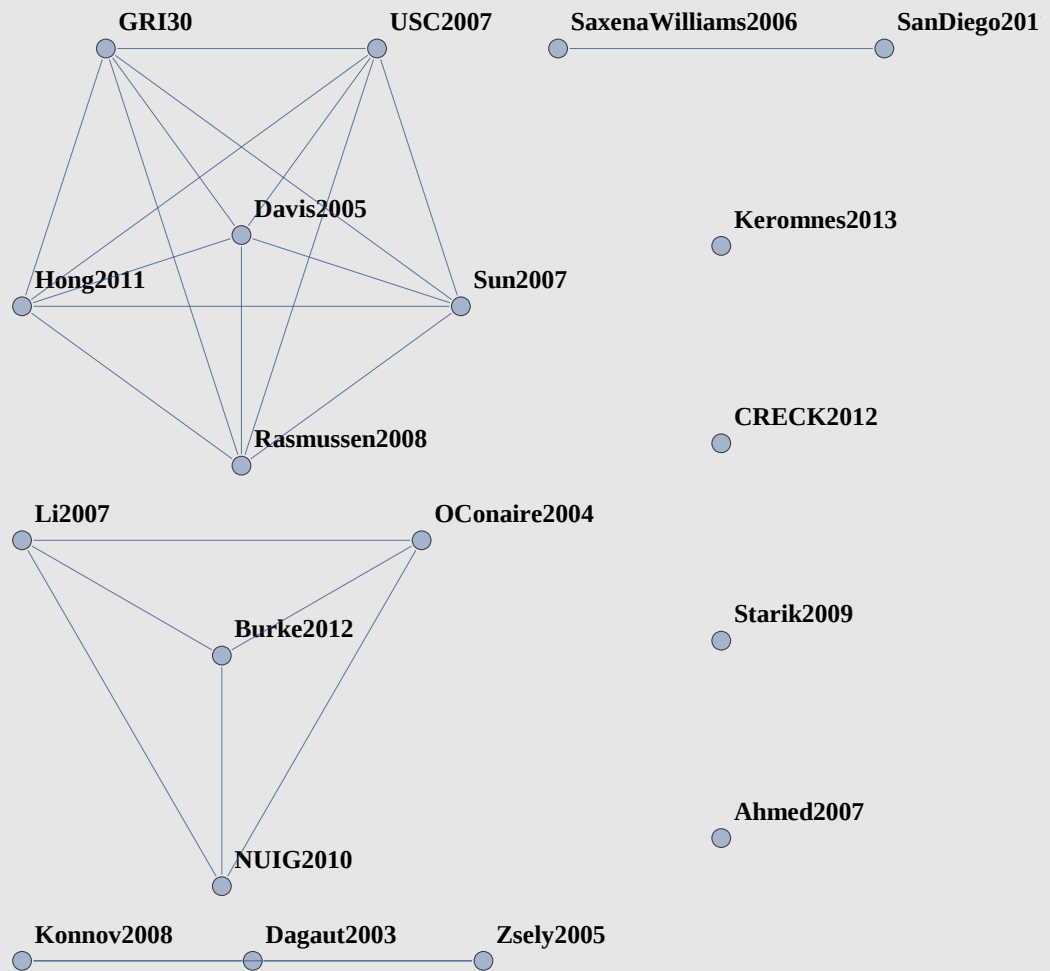
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Burke2012	False	TRUE	False	False	False
CRECK2012	False	False	TRUE	False	False
Dagaut2003	False	False	False	TRUE	False
Davis2005	False	False	False	False	TRUE
GRI30	False	False	False	False	TRUE
Hong2011	False	False	False	False	TRUE
Keromnes2013	False	False	False	False	False
Konnov2008	False	False	False	TRUE	False
Li2007	False	TRUE	False	False	False
NUIG2010	False	TRUE	False	False	False
OConaire2004	False	TRUE	False	False	False
Rasmussen2008	False	False	False	False	TRUE
SanDiego2011	False	False	False	False	False
SaxenaWilliams2006	False	False	False	False	False
Starik2009	False	False	False	False	False
Sun2007	False	False	False	False	TRUE
USC2007	False	False	False	False	TRUE
Zsely2005	False	False	False	TRUE	False

```
TableForm[Table[TrueQ[(hevery[[i, 2]] /. "HV" → 0) == (hevery[[j, 2]] /. "HV" → 0)] /.
  {True → Style["T", Bold, Red], False → Style["F", Bold, Blue]},
  {i, 19}, {j, 19}], TableHeadings → {indices, indices}]
```

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	T	F	F	F	F	F	F	F	F	F	F	F	F	F	F
2	F	T	F	F	F	F	F	F	F	T	T	T	F	F	F
3	F	F	T	F	F	F	F	F	F	F	F	F	F	F	F
4	F	F	F	T	F	F	F	F	T	F	F	F	F	F	F
5	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
6	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
7	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
8	F	F	F	F	F	F	F	T	F	F	F	F	F	F	F
9	F	F	F	T	F	F	F	F	T	F	F	F	F	F	F
10	F	T	F	F	F	F	F	F	F	T	T	T	F	F	F
11	F	T	F	F	F	F	F	F	F	T	T	T	F	F	F
12	F	T	F	F	F	F	F	F	F	T	T	T	F	F	F
13	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
14	F	F	F	F	F	F	F	F	F	F	F	F	F	T	T
15	F	F	F	F	F	F	F	F	F	F	F	F	F	T	T
16	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F
17	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
18	F	F	F	F	T	T	T	F	F	F	F	F	T	F	F
19	F	F	F	T	F	F	F	F	T	F	F	F	F	F	F

```
ag = (tt /. {Style["TRUE", Bold] → 1, False → 0}) - IdentityMatrix[19];
```

```
AdjacencyGraph[ag, ImageSize → 550, ImagePadding → 60, VertexLabels →
  Thread[Rule[indices, Style[#, Bold, 12] & /@ hevery[indices, 3]]]]
```



```
wc = ConnectedComponents[AdjacencyGraph[ag]] /.
  Thread[Rule[indices, hevery[indices, 3]]];
```

```
TableForm[wc, TableHeadings → {Range[8], None}]
```

1	Ahmed2007				
2	Burke2012	Li2007	NUIG2010	OConaire2004	
3	CRECK2012				
4	Dagaut2003	Konnov2008	Zsely2005		
5	Davis2005	GRI30	Hong2011	Rasmussen2008	Sun2006
6	Keromnes2013				
7	SanDiego2011	SaxenaWilliams2006			
8	Starik2009				

```
reducedindices = Sort[First /@ ConnectedComponents[AdjacencyGraph[ag]]]
```

```
{1, 2, 3, 4, 5, 8, 14, 16}
```

```
Column[
  Riffle[Row /@ (Join[{Style[hevery[[#, 3]], Bold, 14], "\t"}, VolpertIndexing[
    hevery[[#, 2]], {"H2", "O2"}, Verbose → True,
    ExternalSpecies → {"HV"}]] & /@ reducedindices), "\n\n"], 2]
```

		Reaction steps	Indices	
		$O_2 \rightarrow 2 O$	0	
		$H_2 + O_2 \rightarrow H + H_2O_2$	0	
		$H_2 \rightarrow 2 H$	0	
		$H + O_2 \rightarrow O + OH$	1	
		$H_2O_2 + O \rightarrow O_2 + OH$	1	
		$H_2 + O \rightarrow H + OH$	1	
		$2 O \rightarrow O_2$	1	
		$H + H_2O_2 \rightarrow 2 OH$	1	
		$H + H_2O_2 \rightarrow H_2 + O_2$	1	
		$H + H_2O_2 \rightarrow H_2O + O$	1	
		$2 H_2O_2 \rightarrow H_2O_2 + O_2$	1	
		$H + O_2 \rightarrow H_2O_2$	1	
		$H_2O_2 \rightarrow H + O_2$	1	
		$H_2 + H_2O_2 \rightarrow H + H_2O_2$	1	
		$2 H \rightarrow H_2$	1	
Ahmed2007	Species	Indices		
	O_2	0	$H_2O_2 + OH \rightarrow H_2O + O_2$	2
	H_2	0	$H_2O + O_2 \rightarrow H_2O_2 + OH$	2
	O	1	$O + OH \rightarrow H + O_2$	2
	H_2O_2	1	$O_2 + OH \rightarrow H_2O_2 + O$	2
	H	1	$H_2O_2 + OH \rightarrow H_2O_2 + O$	2
	H_2O_2	2	$H_2O_2 + O \rightarrow H_2O_2 + OH$	2
	OH	2	$2 OH \rightarrow H_2O + O$	2
	H_2O	2	$H_2O + O \rightarrow 2 OH$	2
			$H + OH \rightarrow H_2 + O$	2
		$H_2O_2 + OH \rightarrow H_2O + H_2O_2$	2	
		$H_2O + H_2O_2 \rightarrow H_2O_2 + OH$	2	
		$2 OH \rightarrow H + H_2O_2$	2	
		$H_2O + O \rightarrow H + H_2O_2$	2	
		$H_2O_2 + O_2 \rightarrow 2 H_2O_2$	2	
		$H_2O + OH \rightarrow H + H_2O_2$	2	
		$H + H_2O_2 \rightarrow H_2O + OH$	2	
		$H + H_2O_2 \rightarrow H_2 + H_2O_2$	2	
		$2 OH \rightarrow H_2O_2$	2	
		$H_2O_2 \rightarrow 2 OH$	2	
		$H_2 + OH \rightarrow H + H_2O$	2	
		$H + H_2O \rightarrow H_2 + OH$	2	
		$H + OH \rightarrow H_2O$	2	
		$H_2O \rightarrow H + OH$	2	

Burke2012

		Reaction steps	Indices
		$O_2 \rightarrow 2 O$	0
		$H_2 + O_2 \rightarrow H + H_2O_2$	0
		$H_2 \rightarrow 2 H$	0
		$H + O_2 \rightarrow O + OH$	1
		$H_2O_2 + O \rightarrow O_2 + OH$	1
		$H_2 + O \rightarrow H + OH$	1
		$H + O \rightarrow OH$	1
		$2 O \rightarrow O_2$	1
		$H + H_2O_2 \rightarrow 2 OH$	1
		$H + H_2O_2 \rightarrow H_2 + O_2$	1
		$2 H_2O_2 \rightarrow H_2O_2 + O_2$	1
		$H + O_2 \rightarrow H_2O_2$	1
		$H_2O_2 \rightarrow H + O_2$	1
		$H_2 + H_2O_2 \rightarrow H + H_2O_2$	1
		$2 H \rightarrow H_2$	1
Species	Indices	$H_2O_2 + OH \rightarrow H_2O + O_2$	2
O_2	0	$O + OH \rightarrow H + O_2$	2
H_2	0	$O_2 + OH \rightarrow H_2O_2 + O$	2
O	1	$H_2O_2 + OH \rightarrow H_2O_2 + O$	2
H_2O_2	1	$H_2O_2 + O \rightarrow H_2O_2 + OH$	2
H	1	$2 OH \rightarrow H_2O + O$	2
H_2O_2	2	$H + OH \rightarrow H_2 + O$	2
OH	2	$OH \rightarrow H + O$	2
H_2O	3	$H_2O_2 + OH \rightarrow H_2O + H_2O_2$	2
		$2 OH \rightarrow H + H_2O_2$	2
		$H_2O_2 + O_2 \rightarrow 2 H_2O_2$	2
		$H + H_2O_2 \rightarrow H_2O + OH$	2
		$H + H_2O_2 \rightarrow H_2 + H_2O_2$	2
		$2 OH \rightarrow H_2O_2$	2
		$H_2O_2 \rightarrow 2 OH$	2
		$H_2 + OH \rightarrow H + H_2O$	2
		$H + OH \rightarrow H_2O$	2
		$H_2O + O_2 \rightarrow H_2O_2 + OH$	3
		$H_2O + O \rightarrow 2 OH$	3
		$H_2O + H_2O_2 \rightarrow H_2O_2 + OH$	3
		$H_2O + OH \rightarrow H + H_2O_2$	3
		$H + H_2O \rightarrow H_2 + OH$	3
		$H_2O \rightarrow H + OH$	3

CRECK2012

		Reaction steps	Indices
		$O_2 \rightarrow 2 O$	0
		$H_2 + O_2 \rightarrow H + HO_2$	0
		$H_2 \rightarrow 2 H$	0
		$H + O_2 \rightarrow O + OH$	1
		$HO_2 + O \rightarrow O_2 + OH$	1
		$H_2 + O \rightarrow H + OH$	1
		$2 O \rightarrow O_2$	1
		$H + HO_2 \rightarrow 2 OH$	1
		$H + HO_2 \rightarrow H_2 + O_2$	1
		$2 HO_2 \rightarrow H_2O_2 + O_2$	1
		$HO_2 \rightarrow O + OH$	1
		$H + O_2 \rightarrow HO_2$	1
		$HO_2 \rightarrow H + O_2$	1
		$H_2 + HO_2 \rightarrow H + H_2O_2$	1
		$2 H \rightarrow H_2$	1
		$HO_2 + OH \rightarrow H_2O + O_2$	2
		$O + OH \rightarrow H + O_2$	2
		$O_2 + OH \rightarrow HO_2 + O$	2
		$2 OH \rightarrow H_2O + O$	2
		$H + OH \rightarrow H_2 + O$	2
		$H_2O_2 + OH \rightarrow H_2O + HO_2$	2
		$2 OH \rightarrow H + HO_2$	2
		$H_2O_2 + O_2 \rightarrow 2 HO_2$	2
		$O + OH \rightarrow HO_2$	2
		$H + H_2O_2 \rightarrow H_2O + OH$	2
		$H + H_2O_2 \rightarrow H_2 + HO_2$	2
		$2 OH \rightarrow H_2O_2$	2
		$H_2O_2 \rightarrow 2 OH$	2
		$H_2 + OH \rightarrow H + H_2O$	2
		$H + OH \rightarrow H_2O$	2
		$H_2O_2 + O \rightarrow HO_2 + OH$	2
		$H_2O + O_2 \rightarrow HO_2 + OH$	3
		$H_2O + O \rightarrow 2 OH$	3
		$H_2O + HO_2 \rightarrow H_2O_2 + OH$	3
		$H_2O + OH \rightarrow H + H_2O_2$	3
		$H + H_2O \rightarrow H_2 + OH$	3
		$H_2O \rightarrow H + OH$	3

Dagaut2003

		Reaction steps	Indices
		$\text{H}_2 + \text{O}_2 \rightarrow 2 \text{OH}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	1
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{OH} \rightarrow \text{H} + \text{O}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$2 \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2\text{O}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2

Davis2005

		Reaction steps	Indices
		$O_2 \rightarrow 2 O$	0
		$H_2 + O_2 \rightarrow H + HO_2$	0
		$H_2 \rightarrow 2 H$	0
		$H + O_2 \rightarrow O + OH$	1
		$HO_2 + O \rightarrow O_2 + OH$	1
		$H_2 + O \rightarrow H + OH$	1
		$H + O \rightarrow OH$	1
		$2 O \rightarrow O_2$	1
		$H + HO_2 \rightarrow 2 OH$	1
		$H + HO_2 \rightarrow H_2 + O_2$	1
		$H + HO_2 \rightarrow H_2O + O$	1
		$2 HO_2 \rightarrow H_2O_2 + O_2$	1
		$H + O_2 \rightarrow HO_2$	1
		$HO_2 \rightarrow H + O_2$	1
		$H_2 + HO_2 \rightarrow H + H_2O_2$	1
		$2 H \rightarrow H_2$	1
		$HO_2 + OH \rightarrow H_2O + O_2$	2
		$H_2O + O_2 \rightarrow HO_2 + OH$	2
		$O + OH \rightarrow H + O_2$	2
		$O_2 + OH \rightarrow HO_2 + O$	2
		$HO_2 + OH \rightarrow H_2O_2 + O$	2
		$H_2O_2 + O \rightarrow HO_2 + OH$	2
		$2 OH \rightarrow H_2O + O$	2
		$H_2O + O \rightarrow 2 OH$	2
		$H + OH \rightarrow H_2 + O$	2
		$OH \rightarrow H + O$	2
		$H_2O_2 + OH \rightarrow H_2O + HO_2$	2
		$H_2O + HO_2 \rightarrow H_2O_2 + OH$	2
		$2 OH \rightarrow H + HO_2$	2
		$H_2O + O \rightarrow H + HO_2$	2
		$H_2O_2 + O_2 \rightarrow 2 HO_2$	2
		$H_2O + OH \rightarrow H + H_2O_2$	2
		$H + H_2O_2 \rightarrow H_2O + OH$	2
		$H + H_2O_2 \rightarrow H_2 + HO_2$	2
		$2 OH \rightarrow H_2O_2$	2
		$H_2O_2 \rightarrow 2 OH$	2
		$H_2 + OH \rightarrow H + H_2O$	2
		$H + H_2O \rightarrow H_2 + OH$	2
		$H + OH \rightarrow H_2O$	2
		$H_2O \rightarrow H + OH$	2

Keromnes2013

		Reaction steps	Indices
		$O_2 \rightarrow 2 O$	0
		$H_2 + O_2 \rightarrow H + H_2O$	0
		$H_2 \rightarrow 2 H$	0
		$H + O_2 \rightarrow O + OH$	1
		$H_2O + O \rightarrow O_2 + OH$	1
		$H_2 + O \rightarrow H + OH$	1
		$H + O \rightarrow OHEX$	1
		$H + O \rightarrow OH$	1
		$2 O \rightarrow O_2$	1
		$H + H_2O \rightarrow 2 OH$	1
		$H + H_2O \rightarrow H_2 + O_2$	1
		$2 H_2O \rightarrow H_2O_2 + O_2$	1
		$H + O_2 \rightarrow H_2O$	1
		$H_2O \rightarrow H + O_2$	1
		$H_2 + H_2O \rightarrow H + H_2O_2$	1
		$2 H \rightarrow H_2$	1
		$OHEX \rightarrow OH$	2
		$OH \rightarrow OHEX$	2
		$H_2O + OH \rightarrow H_2O + O_2$	2
		$O + OH \rightarrow H + O_2$	2
		$O_2 + OH \rightarrow H_2O + O$	2
		$H_2O + OH \rightarrow H_2O_2 + O$	2
		$H_2O_2 + O \rightarrow H_2O + OH$	2
		$2 OH \rightarrow H_2O + O$	2
		$H + OH \rightarrow H_2 + O$	2
		$OHEX \rightarrow H + O$	2
		$OH \rightarrow H + O$	2
		$H_2O_2 + OH \rightarrow H_2O + H_2O$	2
		$2 OH \rightarrow H + H_2O$	2
		$H_2O_2 + O_2 \rightarrow 2 H_2O$	2
		$H + H_2O_2 \rightarrow H_2O + OH$	2
		$H + H_2O_2 \rightarrow H_2 + H_2O$	2
		$2 OH \rightarrow H_2O_2$	2
		$H_2O_2 \rightarrow 2 OH$	2
		$H_2 + OH \rightarrow H + H_2O$	2
		$H + OH \rightarrow H_2O$	2
		$H_2O + O_2 \rightarrow H_2O + OH$	3
		$H_2O + O \rightarrow 2 OH$	3
		$H_2O + H_2O \rightarrow H_2O_2 + OH$	3
		$H_2O + OH \rightarrow H + H_2O_2$	3
		$H + H_2O \rightarrow H_2 + OH$	3
		$H_2O \rightarrow H + OH$	3

SanDiego2011

		Reaction steps	Indices
		$O_2 \rightarrow 2 O$	0
		$H_2 + O_2 \rightarrow H + H_2O$	0
		$H_2 \rightarrow 2 H$	0
		$H + O_2 \rightarrow O + OH$	1
		$H_2O + O \rightarrow O_2 + OH$	1
		$H_2 + O \rightarrow H + OH$	1
		$H + O \rightarrow OH$	1
		$2 O \rightarrow O_2$	1
		$H + H_2O \rightarrow 2 OH$	1
		$H + H_2O \rightarrow H_2 + O_2$	1
		$H + H_2O \rightarrow H_2O + O$	1
		$2 H_2O \rightarrow H_2O_2 + O_2$	1
		$H_2O \rightarrow O + OH$	1
		$H + O_2 \rightarrow H_2O$	1
		$H_2O \rightarrow H + O_2$	1
		$H_2 + H_2O \rightarrow H + H_2O_2$	1
		$2 H \rightarrow H_2$	1
Species	Indices	$H_2O + OH \rightarrow H_2O + O_2$	2
		$H_2O + O_2 \rightarrow H_2O + OH$	2
		$O + OH \rightarrow H + O_2$	2
		$O_2 + OH \rightarrow H_2O + O$	2
		$H_2O + OH \rightarrow H_2O_2 + O$	2
		$H_2O_2 + O \rightarrow H_2O + OH$	2
		$2 OH \rightarrow H_2O + O$	2
		$H_2O + O \rightarrow 2 OH$	2
		$H + OH \rightarrow H_2 + O$	2
		$OH \rightarrow H + O$	2
		$H_2O_2 + OH \rightarrow H_2O + H_2O$	2
		$H_2O + H_2O \rightarrow H_2O_2 + OH$	2
		$2 OH \rightarrow H + H_2O$	2
		$H_2O + O \rightarrow H + H_2O$	2
		$H_2O_2 + O_2 \rightarrow 2 H_2O$	2
		$O + OH \rightarrow H_2O$	2
		$H_2O + OH \rightarrow H + H_2O_2$	2
		$H + H_2O_2 \rightarrow H_2O + OH$	2
		$H + H_2O_2 \rightarrow H_2 + H_2O$	2
		$2 OH \rightarrow H_2O_2$	2
		$H_2O_2 \rightarrow 2 OH$	2
		$H_2 + OH \rightarrow H + H_2O$	2
		$H + H_2O \rightarrow H_2 + OH$	2
		$H + OH \rightarrow H_2O$	2
		$H_2O \rightarrow H + OH$	2

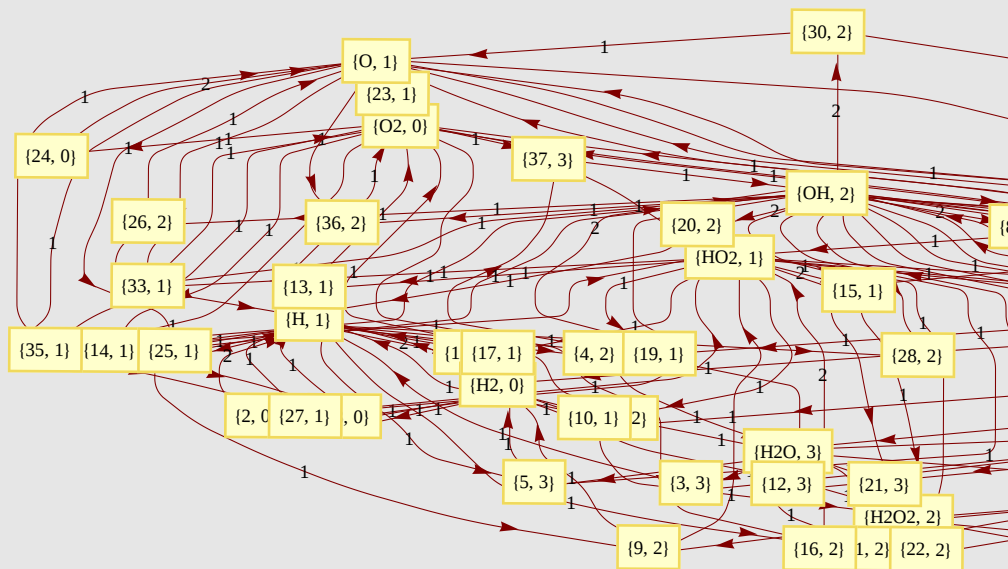
Starik2009

		Reaction steps	Indices
		$2\text{ O}_2 \rightarrow \text{O} + \text{O}_3$	0
		$\text{O}_2 \rightarrow 2\text{ O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	0
		$\text{H}_2 \rightarrow 2\text{ H}$	0
		$\text{H}_2\text{O}_2 + \text{O}_3 \rightarrow 2\text{ O}_2 + \text{OH}$	1
		$\text{H}_2 + \text{O}_3 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	1
		$\text{H} + \text{O}_3 \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{O}_3 \rightarrow \text{O} + \text{O}_2$	1
		$\text{O} + \text{O}_2 \rightarrow \text{O}_3$	1
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow \text{O}_3 + \text{OH}$	1
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{O} + \text{O}_3 \rightarrow 2\text{ O}_2$	1
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$2\text{ O} \rightarrow \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow 2\text{ OH}$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$2\text{ H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2\text{O}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2\text{ H} \rightarrow \text{H}_2$	1
		$2\text{ O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}_3$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2 + \text{O}_3$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{H} + \text{O}_3$	2
		$\text{O}_3 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2\text{ OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2\text{ OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2\text{ OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2\text{ H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O}_2$	2
		$2\text{ OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2\text{ OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2

Species	Indices
O2	0
H2	0
O3	1
O	1
H2O2	1
H	1
H2O2	2
OH	2
H2O	2

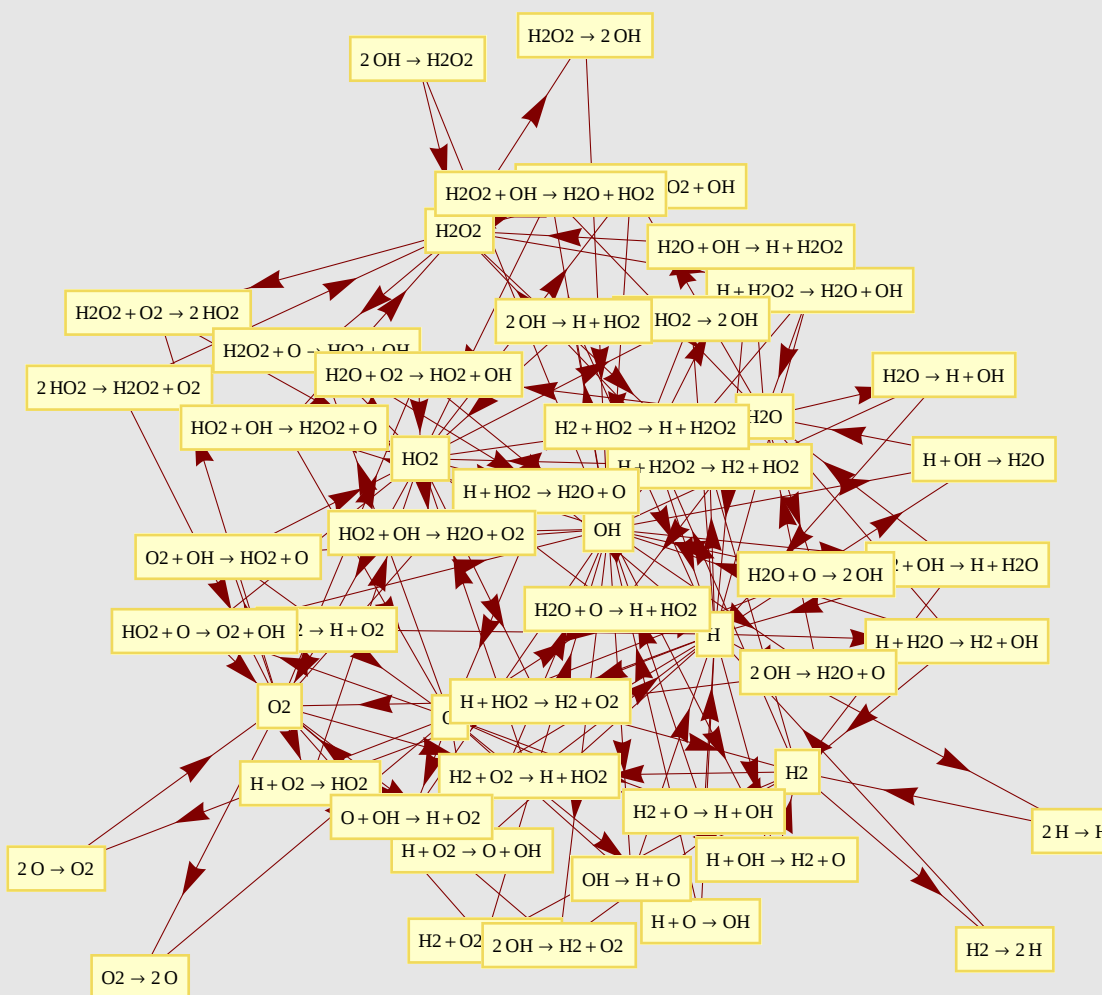
```
ShowVolpertGraph[hevery[[12, 2]], PlotFunction -> "LayeredGraphPlot",
DirectedEdges -> True, VertexLabeling -> True, ImageSize -> 900,
PlotLabel -> Style["Volpert graph of " <> hevery[[12, 3]], 15, Bold, Black],
EdgeLabeling -> True, Numbered -> True, Indexed -> {"H2", "O2"},
MultiedgeStyle -> True, PlotRangeClipping -> True]
```

Volpert graph of OConaire2004



```
ShowVolpertGraph[hevery[[19, 2]], MultiedgeStyle → True,
DirectedEdges → True, VertexLabeling → True,
PlotLabel → Style["Volpert graph of " <> hevery[[19, 3]], 15, Bold, Black],
ImageSize → 600]
```

Volpert graph of Zsely2005



```
ReversibleQ /@ hevery[reducedindices, 2]
```

```
{True, True, False, True, True, True, True, True}
```

```
db = Sort[DetailedBalanced[#, Total[Length /@ (#1 /. Equal → List)] <
Total[Length /@ (#2 /. Equal → List)] &] & /@
hevery[Delete[reducedindices, 3], 2]
```

DetailedBalanced::nocycle :

The FHJ-graph of the given formal mechanism has no cycle, so we are given only the spanning forest condition(s).

$$\begin{aligned}
& \{ \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{19} = k_1 k_{13} k_{20}, k_4 k_{13} k_{37} = k_3 k_{14} k_{38}, \\
& k_{18} k_{21} k_{30} = k_{17} k_{22} k_{29}, k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, k_2 k_8 k_9 k_{21} = k_1 k_7 k_{10} k_{22}, \\
& k_2 k_4 k_9 k_{23} = k_1 k_3 k_{10} k_{24}, k_2 k_4 k_{28} k_{29} = k_1 k_3 k_{27} k_{30}, k_3 k_{14} k_{30} k_{33} = k_4 k_{13} k_{29} k_{34}, \\
& k_1 k_3 k_{10} k_{30} k_{31} = k_2 k_4 k_9 k_{29} k_{32}, k_2 k_4^2 k_8 k_9 k_{13} k_{26} k_{29}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{25} k_{30}^2, \\
& k_2 k_4 k_8 k_9 k_{13} k_{29} k_{35} = k_1 k_3 k_7 k_{10} k_{14} k_{30} k_{36} \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{17} = k_1 k_{13} k_{18}, \\
& k_4 k_{13} k_{37} = k_3 k_{14} k_{38}, k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, k_2 k_8 k_9 k_{19} = k_1 k_7 k_{10} k_{20}, \\
& k_2 k_4 k_9 k_{21} = k_1 k_3 k_{10} k_{22}, k_2 k_8 k_9 k_{13} k_{24} k_{25}^2 = k_1 k_7 k_{10} k_{14} k_{23} k_{26}^2, \\
& k_1 k_8 k_9 k_{13} k_{24} k_{27}^2 = k_2 k_7 k_{10} k_{14} k_{23} k_{28}^2, k_1 k_8 k_{10} k_{13} k_{24} k_{31}^2 = k_2 k_7 k_9 k_{14} k_{23} k_{32}^2, \\
& k_2 k_8 k_9 k_{14} k_{24} k_{33}^2 = k_1 k_7 k_{10} k_{13} k_{23} k_{34}^2, k_2 k_8 k_9 k_{13} k_{23} k_{35}^2 = k_1 k_7 k_{10} k_{14} k_{24} k_{36}^2, \\
& k_2 k_4^2 k_8 k_9 k_{13} k_{24} k_{29}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{23} k_{30}^2 \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_4 k_{28} k_{31} = k_3 k_{27} k_{32}, \\
& k_4 k_{13} k_{41} = k_3 k_{14} k_{42}, k_{20} k_{21} k_{40} = k_{19} k_{22} k_{39}, k_{18} k_{21} k_{32} = k_{17} k_{22} k_{31}, \\
& k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, k_2 k_8 k_9 k_{21} = k_1 k_7 k_{10} k_{22}, k_8 k_9 k_{13} k_{39} = k_7 k_{10} k_{14} k_{40}, \\
& k_2 k_4 k_9 k_{23} = k_1 k_3 k_{10} k_{24}, k_2 k_4 k_{30} k_{31} = k_1 k_3 k_{29} k_{32}, k_3 k_{14} k_{32} k_{35} = k_4 k_{13} k_{31} k_{36}, \\
& k_1 k_3 k_{10} k_{32} k_{33} = k_2 k_4 k_9 k_{31} k_{34}, k_2 k_4^2 k_8 k_9 k_{13} k_{26} k_{31}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{25} k_{32}^2, \\
& k_2 k_4 k_8 k_9 k_{13} k_{31} k_{37} = k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{38} \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{19} = k_1 k_{13} k_{20}, \\
& k_4 k_{28} k_{31} = k_3 k_{27} k_{32}, k_4 k_{13} k_{39} = k_3 k_{14} k_{40}, k_{18} k_{21} k_{32} = k_{17} k_{22} k_{31}, \\
& k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, k_2 k_8 k_9 k_{21} = k_1 k_7 k_{10} k_{22}, k_2 k_4 k_9 k_{23} = k_1 k_3 k_{10} k_{24}, \\
& k_2 k_4 k_{30} k_{31} = k_1 k_3 k_{29} k_{32}, k_3 k_{14} k_{32} k_{35} = k_4 k_{13} k_{31} k_{36}, \\
& k_1 k_3 k_{10} k_{32} k_{33} = k_2 k_4 k_9 k_{31} k_{34}, k_2 k_4^2 k_8 k_9 k_{13} k_{26} k_{31}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{25} k_{32}^2, \\
& k_2 k_4 k_8 k_9 k_{13} k_{31} k_{37} = k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{38} \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{17} = k_1 k_{13} k_{18}, k_4 k_{13} k_{39} = k_3 k_{14} k_{40}, \\
& k_{26} k_{27} k_{42} = k_{25} k_{28} k_{41}, k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, k_2 k_8 k_9 k_{19} = k_1 k_7 k_{10} k_{20}, \\
& k_2 k_4 k_9 k_{21} = k_1 k_3 k_{10} k_{22}, k_2 k_8 k_9 k_{13} k_{24} k_{25}^2 = k_1 k_7 k_{10} k_{14} k_{23} k_{26}^2, \\
& k_1 k_8 k_9 k_{13} k_{24} k_{29}^2 = k_2 k_7 k_{10} k_{14} k_{23} k_{30}^2, k_1 k_8 k_{10} k_{13} k_{24} k_{33}^2 = k_2 k_7 k_9 k_{14} k_{23} k_{34}^2, \\
& k_2 k_8 k_9 k_{14} k_{24} k_{35}^2 = k_1 k_7 k_{10} k_{13} k_{23} k_{36}^2, k_2 k_8 k_9 k_{13} k_{23} k_{37}^2 = k_1 k_7 k_{10} k_{14} k_{24} k_{38}^2, \\
& k_2 k_4^2 k_8 k_9 k_{13} k_{24} k_{31}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{23} k_{32}^2 \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{21} = k_1 k_{13} k_{22}, \\
& k_8 k_{15} k_{35} = k_7 k_{16} k_{36}, k_4 k_{13} k_{41} = k_3 k_{14} k_{42}, k_{20} k_{23} k_{34} = k_{19} k_{24} k_{33}, \\
& k_{14} k_{15} k_{40} = k_{13} k_{16} k_{39}, k_2 k_9 k_{14} k_{17} = k_1 k_{10} k_{13} k_{18}, k_2 k_8 k_9 k_{23} = k_1 k_7 k_{10} k_{24}, \\
& k_2 k_4 k_9 k_{25} = k_1 k_3 k_{10} k_{26}, k_8 k_9 k_{15} k_{31} = k_7 k_{10} k_{16} k_{32}, \\
& k_2 k_8 k_9 k_{15} k_{29} = k_1 k_7 k_{10} k_{16} k_{30}, k_2 k_4 k_8 k_9 k_{15} k_{33} = k_1 k_3 k_7 k_{10} k_{16} k_{34}, \\
& k_2 k_8 k_9 k_{14} k_{15}^2 k_{27} = k_1 k_7 k_{10} k_{13} k_{16}^2 k_{28}, k_2 k_8 k_9 k_{14} k_{15} k_{37} = k_1 k_7 k_{10} k_{13} k_{16} k_{38} \}, \\
& \{ k_2 k_4 k_5 = k_1 k_3 k_6, k_3 k_8 k_{11} = k_4 k_7 k_{12}, k_2 k_{14} k_{19} = k_1 k_{13} k_{20}, k_4 k_{28} k_{31} = k_3 k_{27} k_{32}, \\
& k_4 k_{13} k_{41} = k_3 k_{14} k_{42}, k_{18} k_{21} k_{32} = k_{17} k_{22} k_{31}, k_2 k_9 k_{14} k_{15} = k_1 k_{10} k_{13} k_{16}, \\
& k_2 k_8 k_9 k_{21} = k_1 k_7 k_{10} k_{22}, k_2 k_4 k_9 k_{23} = k_1 k_3 k_{10} k_{24}, k_2 k_4 k_{30} k_{31} = k_1 k_3 k_{29} k_{32}, \\
& k_3 k_{14} k_{32} k_{35} = k_4 k_{13} k_{31} k_{36}, k_1 k_3 k_{10} k_{32} k_{33} = k_2 k_4 k_9 k_{31} k_{34}, \\
& k_3 k_{14} k_{32} k_{38} k_{43} = k_4 k_{13} k_{31} k_{37} k_{44}, k_2 k_4^2 k_8 k_9 k_{13} k_{26} k_{31}^2 = k_1 k_3^2 k_7 k_{10} k_{14} k_{25} k_{32}^2, \\
& k_2 k_4 k_8 k_9 k_{13} k_{31} k_{39} = k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{40}, \\
& k_4 k_8 k_9 k_{13}^2 k_{31} k_{37} k_{49} = k_3 k_7 k_{10} k_{14}^2 k_{32} k_{38} k_{50}, \\
& k_2 k_4 k_8 k_9 k_{31} k_{37} k_{51} = k_1 k_3 k_7 k_{10} k_{32} k_{38} k_{52}, k_1 k_3^2 k_7 k_{10} k_{14} k_{32}^2 k_{38} k_{45} = \\
& k_2 k_4^2 k_8 k_9 k_{13} k_{31}^2 k_{37} k_{46}, k_2 k_4 k_8 k_9 k_{13} k_{31} k_{37} k_{47} = k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{38} k_{48} \} \}
\end{aligned}$$

TableForm[db, TableHeadings → {hevery[Delete[reducedindices, 3], 3]}]

Ahmed2007	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{19} = k_1 k_{13} k_{20}$	k_4
Burke2012	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{17} = k_1 k_{13} k_{18}$	k_4
Dagaut2003	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_4 k_{28} k_{31} = k_3 k_{27} k_{32}$	k_4
Davis2005	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{19} = k_1 k_{13} k_{20}$	k_4
Keromnes2013	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{17} = k_1 k_{13} k_{18}$	k_4
SanDiego2011	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{21} = k_1 k_{13} k_{22}$	k_4
Starik2009	$k_2 k_4 k_5 = k_1 k_3 k_6$	$k_3 k_8 k_{11} = k_4 k_7 k_{12}$	$k_2 k_{14} k_{19} = k_1 k_{13} k_{20}$	k_4

```
TableForm[Table[
  Complement[ReactionsData[hevery[[i, 2]], ExternalSpecies → "HV"] ["fhjgraph"],
    ReactionsData[hevery[[j, 2]], ExternalSpecies → "HV"] ["fhjgraph"]],
  {i, reducedindices}, {j, reducedindices}],
TableHeadings → {hevery[[reducedindices, 3]], hevery[[reducedindices, 3]]}]
```

	Ahmed2007	Burke2012	CRECK2012	
Ahmed2007		H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂	H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂ H ₂ O ₂ + OH → H ₂ O ₂ + O	
Burke2012	H + O → OH OH → H + O		H + O → OH OH → H + O H ₂ O ₂ + OH → H ₂ O ₂ + O	
CRECK2012	H ₂ O ₂ → O + OH O + OH → H ₂ O ₂	H ₂ O ₂ → O + OH O + OH → H ₂ O ₂		
Dagaut2003	H + O → OH H ₂ + O ₂ → 2 OH OH → H + O 2 OH → H ₂ + O ₂	H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂ H ₂ + O ₂ → 2 OH 2 OH → H ₂ + O ₂	H + H ₂ O ₂ → H ₂ O + O H + O → OH H ₂ O + O → H + H ₂ O ₂ H ₂ + O ₂ → 2 OH OH → H + O 2 OH → H ₂ + O ₂ H ₂ O ₂ + OH → H ₂ O ₂ + O	
Davis2005	H + O → OH OH → H + O	H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂	H + H ₂ O ₂ → H ₂ O + O H + O → OH H ₂ O + O → H + H ₂ O ₂ OH → H + O H ₂ O ₂ + OH → H ₂ O ₂ + O	
Keromnes2013	H + O → OH H + O → OHEX OH → H + O OH → OHEX OHEX → H + O OHEX → OH	H + O → OHEX OH → OHEX OHEX → H + O OHEX → OH	H + O → OH H + O → OHEX OH → H + O OH → OHEX H ₂ O ₂ + OH → H ₂ O ₂ + O OHEX → H + O OHEX → OH	
SanDiego2011	H ₂ O ₂ → O + OH H + O → OH OH → H + O O + OH → H ₂ O ₂	H ₂ O ₂ → O + OH H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂ O + OH → H ₂ O ₂	H + H ₂ O ₂ → H ₂ O + O H + O → OH H ₂ O + O → H + H ₂ O ₂ OH → H + O H ₂ O ₂ + OH → H ₂ O ₂ + O	
Starik2009	H + O → OH 2 O ₂ → O + O ₃ H ₂ O ₂ + O ₂ → O ₃ + OH O + O ₂ → O ₃ O ₃ → O + O ₂ H + O ₃ → O ₂ + OH H ₂ + O ₃ → H ₂ O ₂ + OH H ₂ O ₂ + O ₃ → 2 O ₂ + OH O + O ₃ → 2 O ₂ OH → H + O H ₂ O ₂ + OH → H ₂ + O ₃ O ₂ + OH → H + O ₃ 2 O ₂ + OH → H ₂ O ₂ + O ₃ O ₃ + OH → H ₂ O ₂ + O ₂	H + H ₂ O ₂ → H ₂ O + O H ₂ O + O → H + H ₂ O ₂ 2 O ₂ → O + O ₃ H ₂ O ₂ + O ₂ → O ₃ + OH O + O ₂ → O ₃ O ₃ → O + O ₂ H + O ₃ → O ₂ + OH H ₂ + O ₃ → H ₂ O ₂ + OH H ₂ O ₂ + O ₃ → 2 O ₂ + OH O + O ₃ → 2 O ₂ H ₂ O ₂ + OH → H ₂ + O ₃ O ₂ + OH → H + O ₃ 2 O ₂ + OH → H ₂ O ₂ + O ₃ O ₃ + OH → H ₂ O ₂ + O ₂	H + H ₂ O ₂ → H ₂ O + O H + O → OH H ₂ O + O → H + H ₂ O ₂ 2 O ₂ → O + O ₃ H ₂ O ₂ + O ₂ → O ₃ + OH O + O ₂ → O ₃ O ₃ → O + O ₂ H + O ₃ → O ₂ + OH H ₂ + O ₃ → H ₂ O ₂ + OH H ₂ O ₂ + O ₃ → 2 O ₂ + OH O + O ₃ → 2 O ₂ OH → H + O H ₂ O ₂ + OH → H ₂ O ₂ + O H ₂ O ₂ + OH → H ₂ + O ₃ O ₂ + OH → H + O ₃ 2 O ₂ + OH → H ₂ O ₂ + O ₃ O ₃ + OH → H ₂ O ₂ + O ₂	2 (H O + O ₃ H + H ₂ H ₂ O + H ₂ O ₂ 2 (H O ₃

```
TableForm[Table[Length@Complement[
  ReactionsData[hevery[[i, 2]], ExternalSpecies → "HV"] ["fhjgraph"],
  ReactionsData[hevery[[j, 2]], ExternalSpecies → "HV"] ["fhjgraph"]],
{i, reducedindices}, {j, reducedindices}],
TableHeadings → {hevery[reducedindices, 3], hevery[reducedindices, 3]}]
```

	Ahmed2007	Burke2012	CRECK2012	Dagaut2003	Davis2005
Ahmed2007	0	2	3	0	0
Burke2012	2	0	3	0	0
CRECK2012	2	2	0	2	2
Dagaut2003	4	4	7	0	2
Davis2005	2	2	5	0	0
Keromnes2013	6	4	7	4	4
SanDiego2011	4	4	5	2	2
Starik2009	14	14	17	12	12

Carbon monoxide combustion mechanisms

```
SetDirectory[NotebookDirectory[] <> "C0"];
```

```
ClearAll[codat, codata];
codat = Flatten[Import["names_C0.txt", "Table"]];
codata = StringReplace[#, ".dat" → ""] & /@ codat

{Ahmed2007, CRECK2012, Dagaut2003, Davis2005, gri30,
Keromnes2013, Li2007, NUIG2010, Rasmussen2008, SanDiego2011,
SaxenaWilliams2006, Starik2009, Sun2007, USC2007, Zsely2005}
```

```
indices = Range[15];
```

```
TableForm[codata, TableHeadings → {indices, None}]
```

1	Ahmed2007
2	CRECK2012
3	Dagaut2003
4	Davis2005
5	gri30
6	Keromnes2013
7	Li2007
8	NUIG2010
9	Rasmussen2008
10	SanDiego2011
11	SaxenaWilliams2006
12	Starik2009
13	Sun2007
14	USC2007
15	Zsely2005

```
ClearAll[coall];
coall = CHEMKINImport[#] ["chemkinreactions"] & /@ codat; // AbsoluteTiming

{2.3421339, Null}
```

```
ClearAll[coevery];
coevery = Transpose[{coall, DeleteAutocatalysis /@ coall, codata}]; //
AbsoluteTiming

{0.6750386, Null}
```

```
TableForm[
  ReactionsData[#, ExternalSpecies → "HV"] ["M", "R", "deficiency"] & /@
    coevery[[indices, 2]],
  TableHeadings → {coevery[[indices, 3]], {"M", "R", "deficiency"}}]
```

	M	R	deficiency
Ahmed2007	12	72	$\delta=n-l-s=57-23-9=25$
CRECK2012	11	60	$\delta=n-l-s=49-19-8=22$
Dagaut2003	12	68	$\delta=n-l-s=52-21-9=22$
Davis2005	11	60	$\delta=n-l-s=47-19-8=20$
gri30	12	74	$\delta=n-l-s=57-23-9=25$
Keromnes2013	12	64	$\delta=n-l-s=52-21-9=22$
Li2007	12	78	$\delta=n-l-s=61-24-9=28$
NUIG2010	12	78	$\delta=n-l-s=61-24-9=28$
Rasmussen2008	13	88	$\delta=n-l-s=66-26-10=30$
SanDiego2011	12	74	$\delta=n-l-s=57-23-9=25$
SaxenaWilliams2006	11	60	$\delta=n-l-s=45-18-8=19$
Starik2009	13	88	$\delta=n-l-s=70-28-10=32$
Sun2007	12	66	$\delta=n-l-s=52-21-9=22$
USC2007	12	74	$\delta=n-l-s=57-23-9=25$
Zsely2005	11	62	$\delta=n-l-s=47-19-8=20$

```
TableForm[ReactionsData[#, ExternalSpecies → {"HV"}][["species"] & /@
  coevery[[indices, 2]],
  TableHeadings → {coevery[[indices, 3]], {"list", " of ", "species\n"}}]
```

	list	of	species					
Ahmed2007	CH2O	H	HCO	CO	CO2	O	H2	OH
CRECK2012	HCO	H2O	CO2	H	OH	H2O2	O	CO
Dagaut2003	CH2O	CO	HCO	CO2	O	H	H2	OH
Davis2005	CO2	CO	O	H	H2	HCO	OH	H2O
gri30	CH2O	CO	H2	H	HCO	CO2	O	OH
Keromnes2013	HCO	CO	H2	H2O	CO2	H	OH	O
Li2007	CH2O	CO	H2	H	HCO	CO2	O	OH
NUIG2010	CH2O	CO	H2	H	HCO	CO2	O	OH
Rasmussen2008	CH2O	CO	H2	H	HCO	CO2	O	H2O
SanDiego2011	CH2O	H	HCO	CO2	CO	O	H2	OH
SaxenaWilliams2006	H	H2	CO	HCO	CO2	O	OH	H2O
Starik2009	CH2O	H	HCO	CO	CO2	O	H2	OH
Sun2007	CH2O	CO	HCO	CO2	O	H	H2	OH
USC2007	CH2O	CO	H2	H	HCO	CO2	O	OH
Zsely2005	CO2	CO	O	H	H2	HCO	OH	H2O

```
TableForm[Table[coevery[[i, 2]] /. x_Equilibrium → Sequence[], {i, 15}],
  TableHeadings → {coevery[[indices, 3]], None}]
```

Ahmed2007		
CRECK2012	$\text{HCO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O} + \text{OH}$
Dagaut2003		
Davis2005		
gri30		
Keromnes2013	$2 \text{HCO} \rightarrow 2 \text{CO} + \text{H}_2$	$\text{HCO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H} + \text{OH}$
Li2007		
NUIG2010		
Rasmussen2008		
SanDiego2011		
SaxenaWilliams2006		
Starik2009		
Sun2007		
USC2007		
Zsely2005		

```
coevery[[2, 2]] /. x_Equilibrium → Sequence[]
```

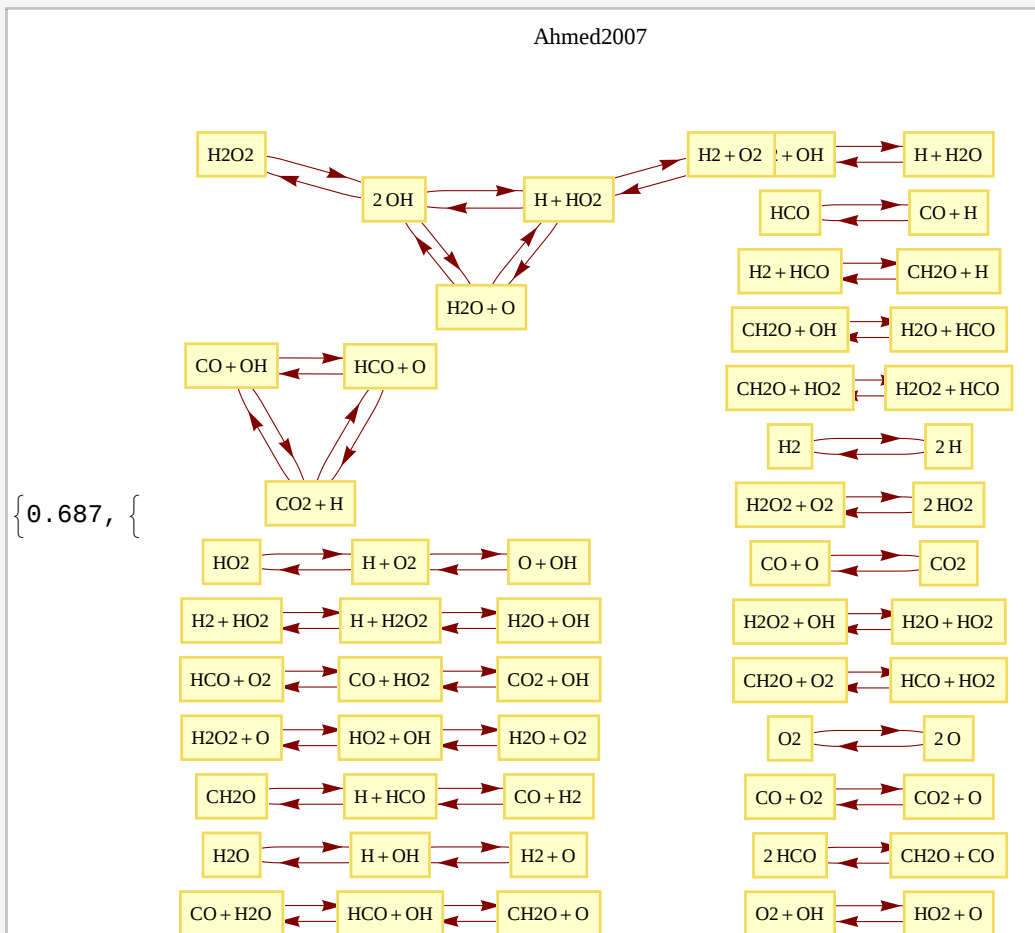
```
{HCO + H2O → CO2 + H + OH, H2O2 + O → H2O + OH}
```

```
coevery[[6, 2]] /. x_Equilibrium → Sequence[]
```

```
{2 HCO → 2 CO + H2, HCO + H2O → CO2 + H + OH}
```

```
Row[{ShowFHJGraph[#[[2]], DirectedEdges → True,
  VertexLabeling → All, PlotLabel → #[[3]], ImageSize → 420], " ",
Column[Join[{"3rd body species deleted"}, #[[2]]], " ", Column[
  Join[{"Orig. Mechanism"}, #[[1]]]]] & /@coevery[indices] // Timing
```

A very large output was generated. Here is a sample of it:



3rd body species deleted

$\text{CH}_2\text{O} \rightleftharpoons \text{H} + \text{HCO}$

$\text{CH}_2\text{O} + \text{CO} \rightleftharpoons 2 \text{HCO}$

$\text{CO}_2 \rightleftharpoons \text{CO} + \text{O}$

$2 \text{H} \rightleftharpoons \text{H}_2$

$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{H}_2 + \text{HCO}$

$\text{CO} + \text{H} \rightleftharpoons \text{HCO}$

$\text{CO}_2 + \text{H} \rightleftharpoons \text{HCO} + \text{O}$

$\text{CO}_2 + \text{H} \rightleftharpoons \text{CO} + \text{OH}$

$\text{CO} + \text{H}_2 \rightleftharpoons \text{H} + \text{HCO}$

$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$

$\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{HCO} + \text{OH}$

$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$

$\text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$

$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$

$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$

$\text{H}_2\text{O} + \text{HCO} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$

Orig. Mechanism

$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$

$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$

$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$

$2 \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$

$\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2$

$\text{H} + \text{HO}_2 \rightleftharpoons 2 \text{OH}$

$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$

$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$

$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$

$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$

$2 \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$

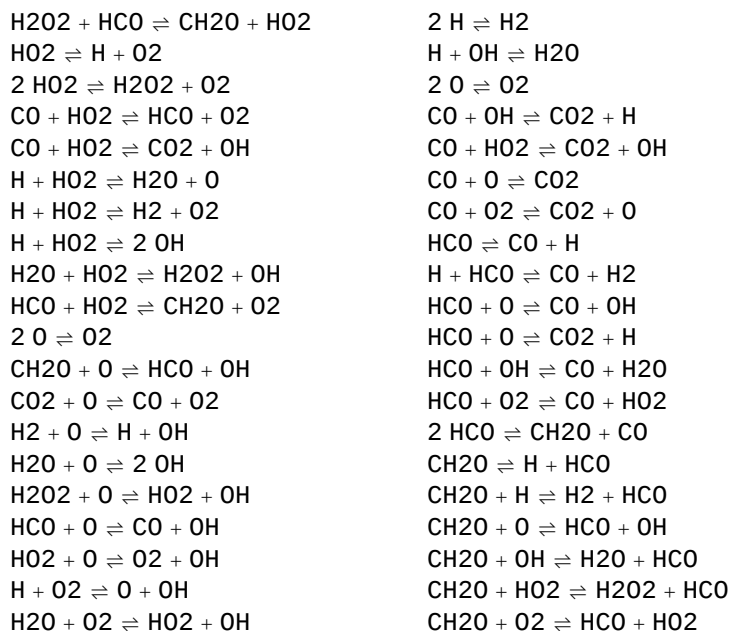
$2 \text{OH} \rightleftharpoons \text{H}_2\text{O}_2$

$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$

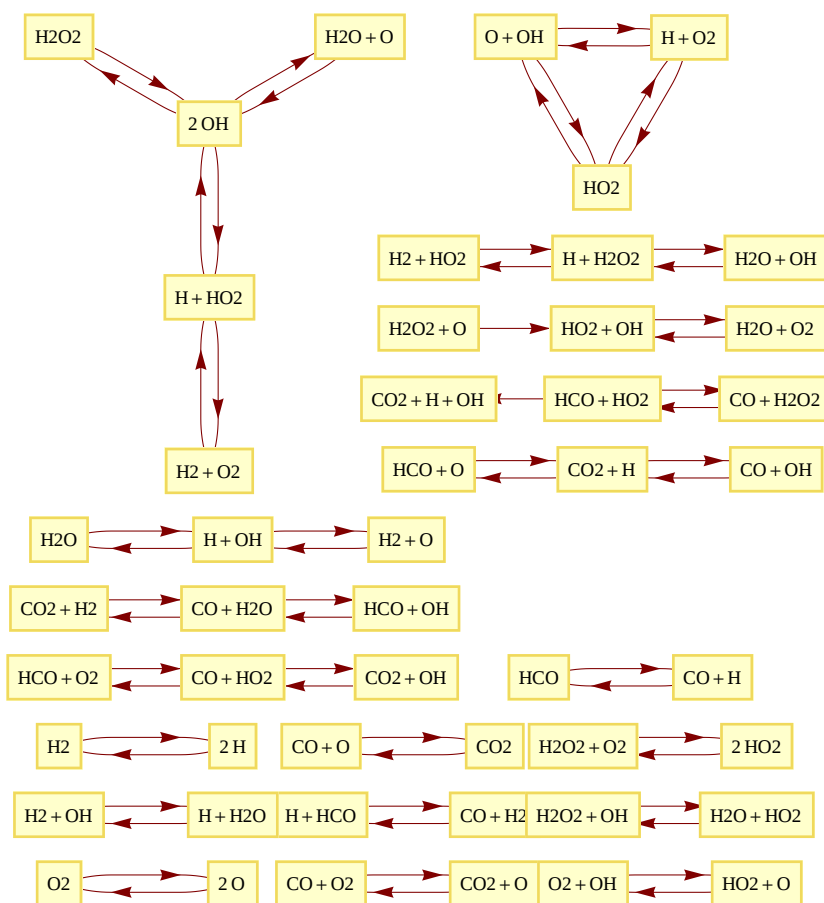
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$

$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$

$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$

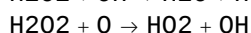
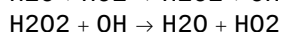
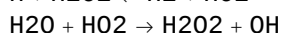
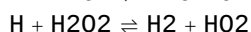
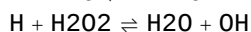
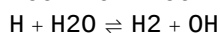
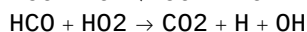
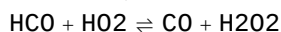
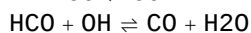
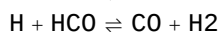
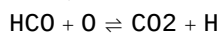
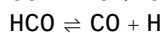
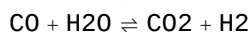
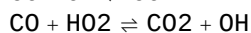
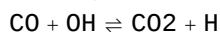
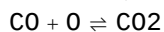
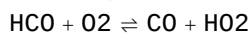
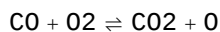
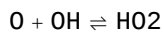
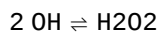
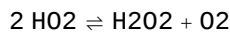
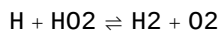
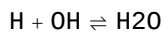
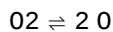
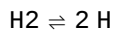
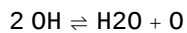
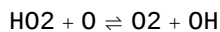
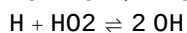
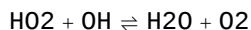
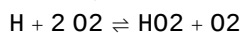
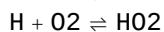
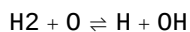
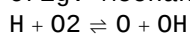
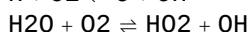
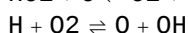
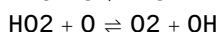
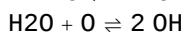
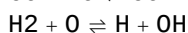
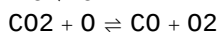
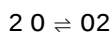
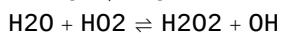
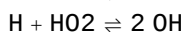
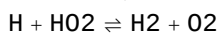
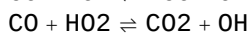
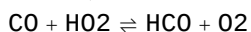
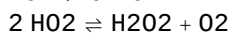
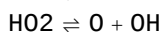
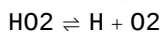
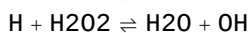
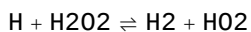
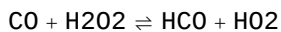
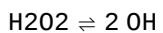
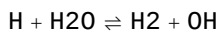
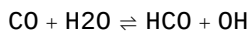
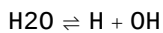
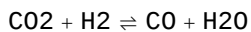
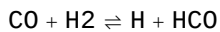
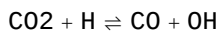
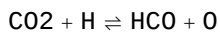
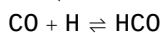
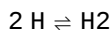
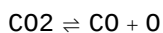
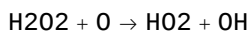
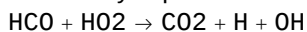


CRECK2012

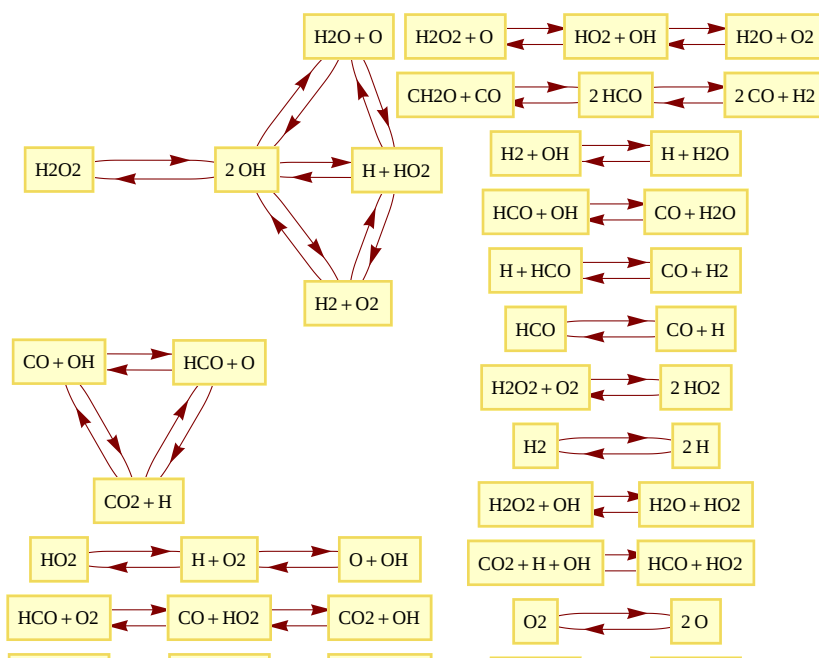


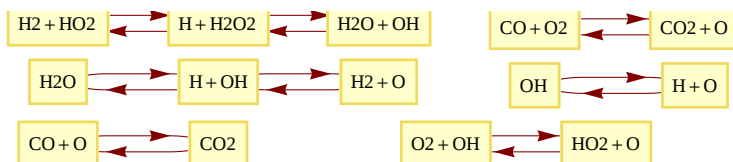
Oria. Mechanism

3rd body species deleted



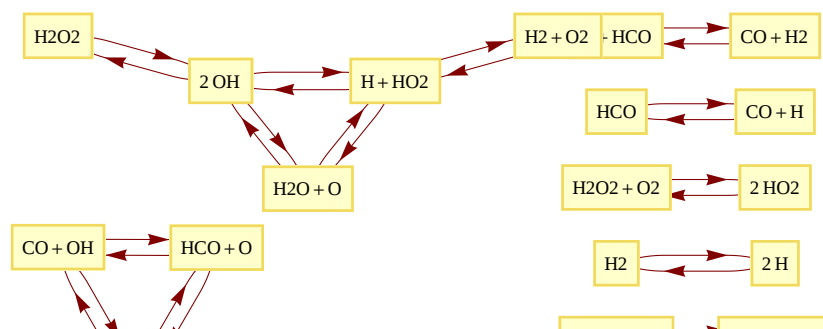
Dagaut2003

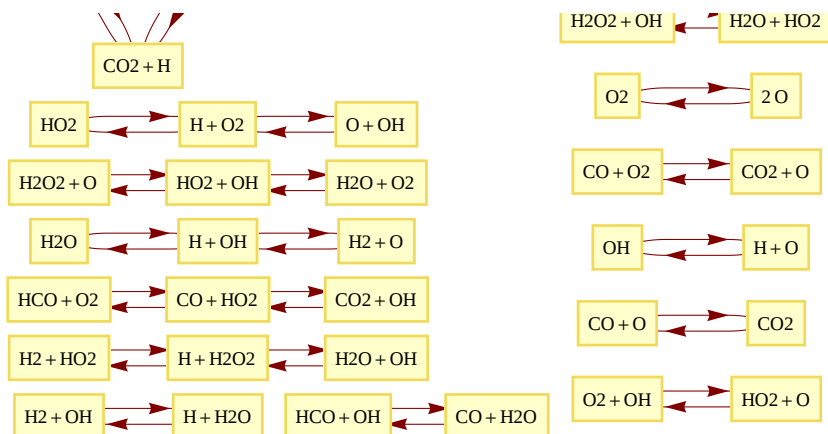




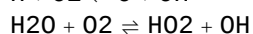
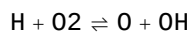
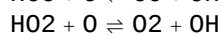
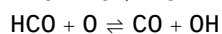
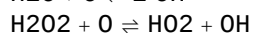
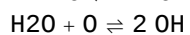
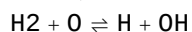
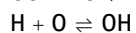
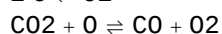
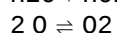
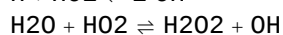
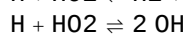
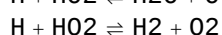
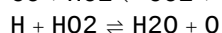
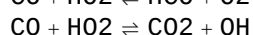
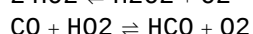
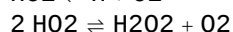
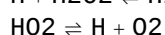
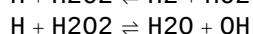
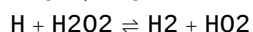
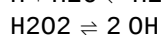
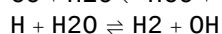
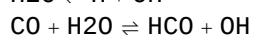
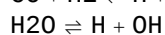
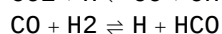
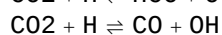
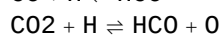
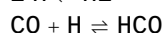
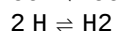
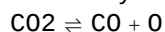
3rd body species deleted	Orig. Mechanism
CH ₂ O + CO ⇌ 2 HCO	2 H ⇌ H ₂
CO ₂ ⇌ CO + O	2 O ⇌ O ₂
2 H ⇌ H ₂	H + O ⇌ OH
CO + H ⇌ HCO	H ₂ + O ₂ ⇌ 2 OH
CO ₂ + H ⇌ HCO + O	H ₂ + O ⇌ H + OH
CO ₂ + H ⇌ CO + OH	H + O ₂ ⇌ O + OH
CO + H ₂ ⇌ H + HCO	H + O ₂ ⇌ HO ₂
2 CO + H ₂ ⇌ 2 HCO	H + OH ⇌ H ₂ O
H ₂ O ⇌ H + OH	H ₂ + OH ⇌ H + H ₂ O
CO + H ₂ O ⇌ HCO + OH	H ₂ O + O ⇌ 2 OH
H + H ₂ O ⇌ H ₂ + OH	HO ₂ + OH ⇌ H ₂ O + O ₂
H ₂ O ₂ ⇌ 2 OH	HO ₂ + O ⇌ O ₂ + OH
H + H ₂ O ₂ ⇌ H ₂ + HO ₂	H + HO ₂ ⇌ H ₂ + O ₂
H + H ₂ O ₂ ⇌ H ₂ O + OH	H + HO ₂ ⇌ 2 OH
HO ₂ ⇌ H + O ₂	H + HO ₂ ⇌ H ₂ O + O
2 HO ₂ ⇌ H ₂ O ₂ + O ₂	2 HO ₂ ⇌ H ₂ O ₂ + O ₂
CO + HO ₂ ⇌ HCO + O ₂	2 OH ⇌ H ₂ O ₂
CO + HO ₂ ⇌ CO ₂ + OH	H ₂ O ₂ + OH ⇌ H ₂ O + HO ₂
H + HO ₂ ⇌ H ₂ O + O	H + H ₂ O ₂ ⇌ H ₂ + HO ₂
H + HO ₂ ⇌ H ₂ + O ₂	H + H ₂ O ₂ ⇌ H ₂ O + OH
H + HO ₂ ⇌ 2 OH	H ₂ O ₂ + O ⇌ HO ₂ + OH
H ₂ O + HO ₂ ⇌ H ₂ O ₂ + OH	CO + HO ₂ ⇌ CO ₂ + OH
HCO + HO ₂ ⇌ CO ₂ + H + OH	CO + OH ⇌ CO ₂ + H
2 O ⇌ O ₂	CO + O ⇌ CO ₂
CO ₂ + O ⇌ CO + O ₂	CO + O ₂ ⇌ CO ₂ + O
H + O ⇌ OH	HCO ⇌ CO + H
H ₂ + O ⇌ H + OH	HCO + OH ⇌ CO + H ₂ O
H ₂ O + O ⇌ 2 OH	HCO + O ⇌ CO + OH
H ₂ O ₂ + O ⇌ HO ₂ + OH	HCO + O ⇌ CO ₂ + H
HCO + O ⇌ CO + OH	H + HCO ⇌ CO + H ₂
HO ₂ + O ⇌ O ₂ + OH	HCO + O ₂ ⇌ CO + HO ₂
H + O ₂ ⇌ O + OH	HCO + HO ₂ ⇌ CO ₂ + H + OH
H ₂ + O ₂ ⇌ 2 OH	2 HCO ⇌ CH ₂ O + CO
H ₂ O + O ₂ ⇌ HO ₂ + OH	2 HCO ⇌ 2 CO + H ₂

Davis2005

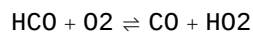
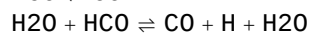
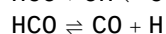
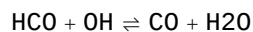
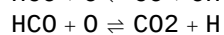
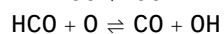
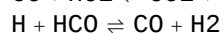
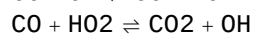
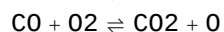
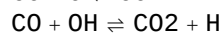
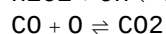
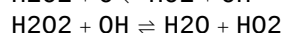
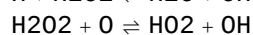
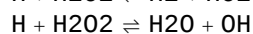
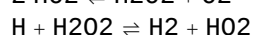
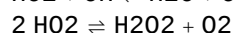
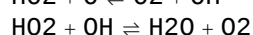
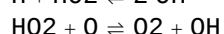
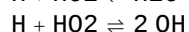
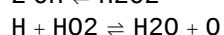
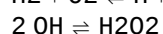
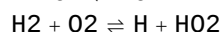
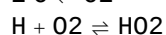
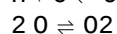
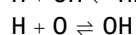
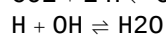
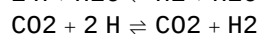
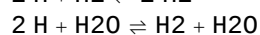
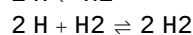
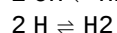
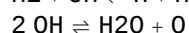
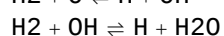
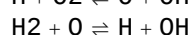
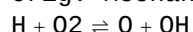




3rd body species deleted

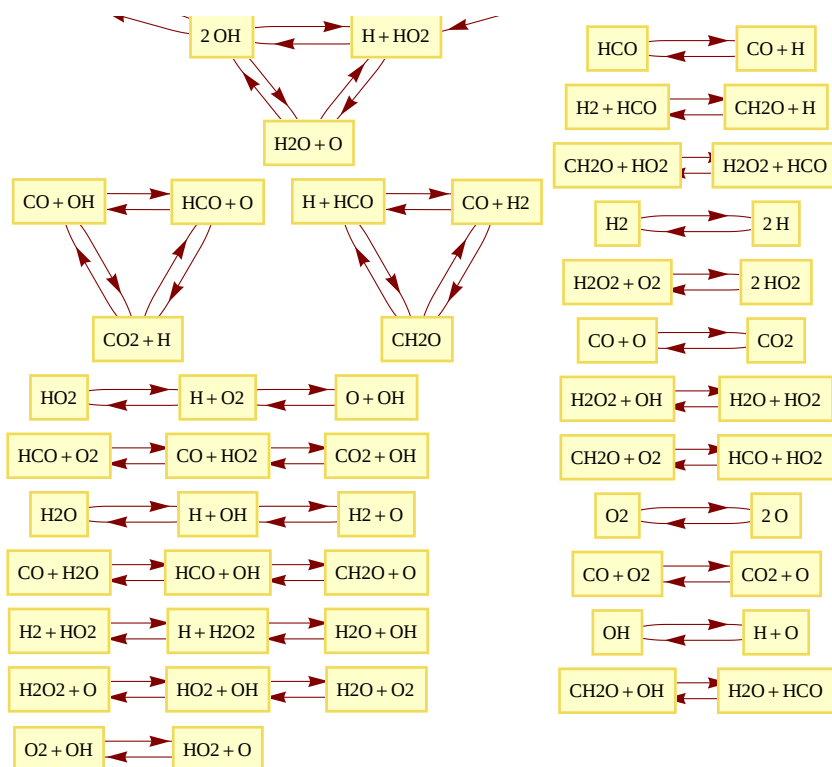


Orig. Mechanism

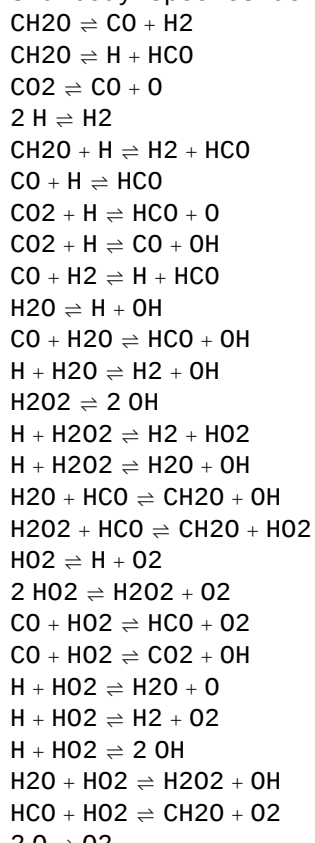


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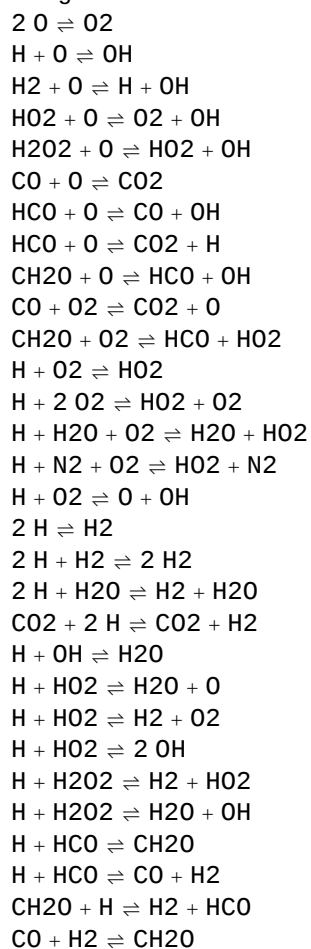


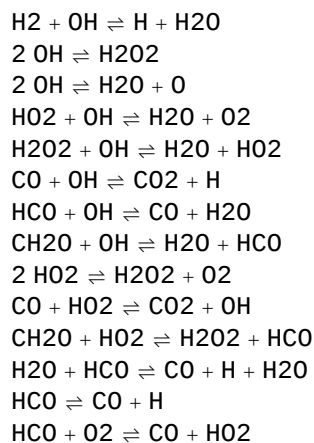
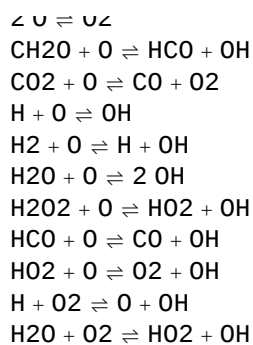


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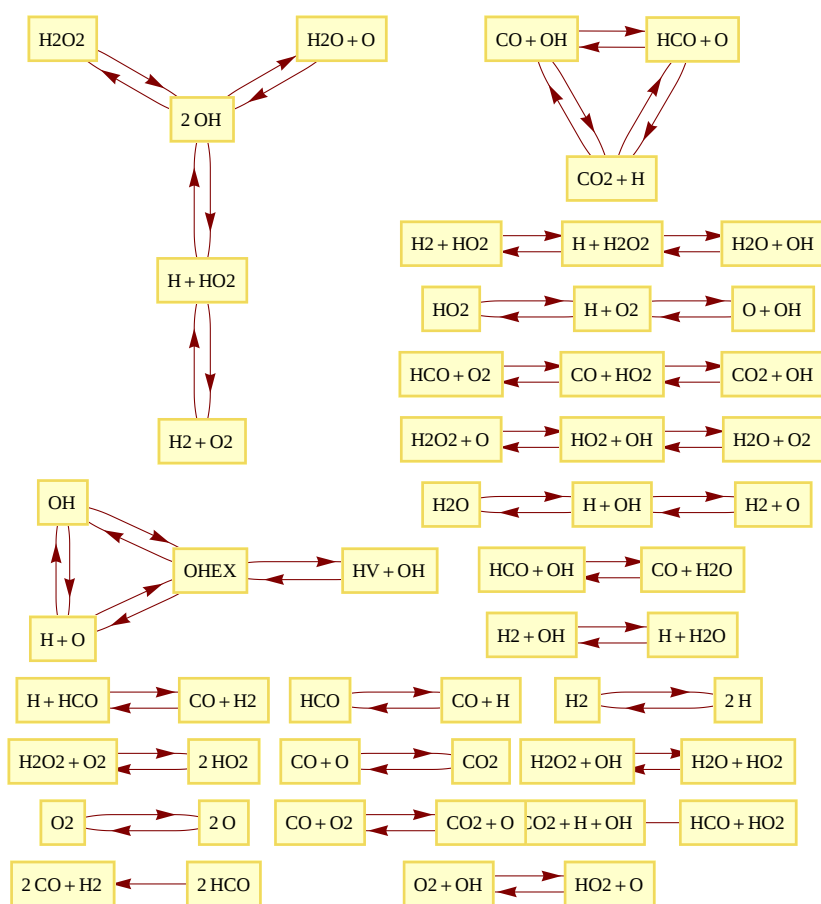


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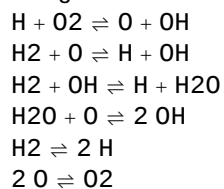




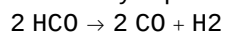
Keromnes2013



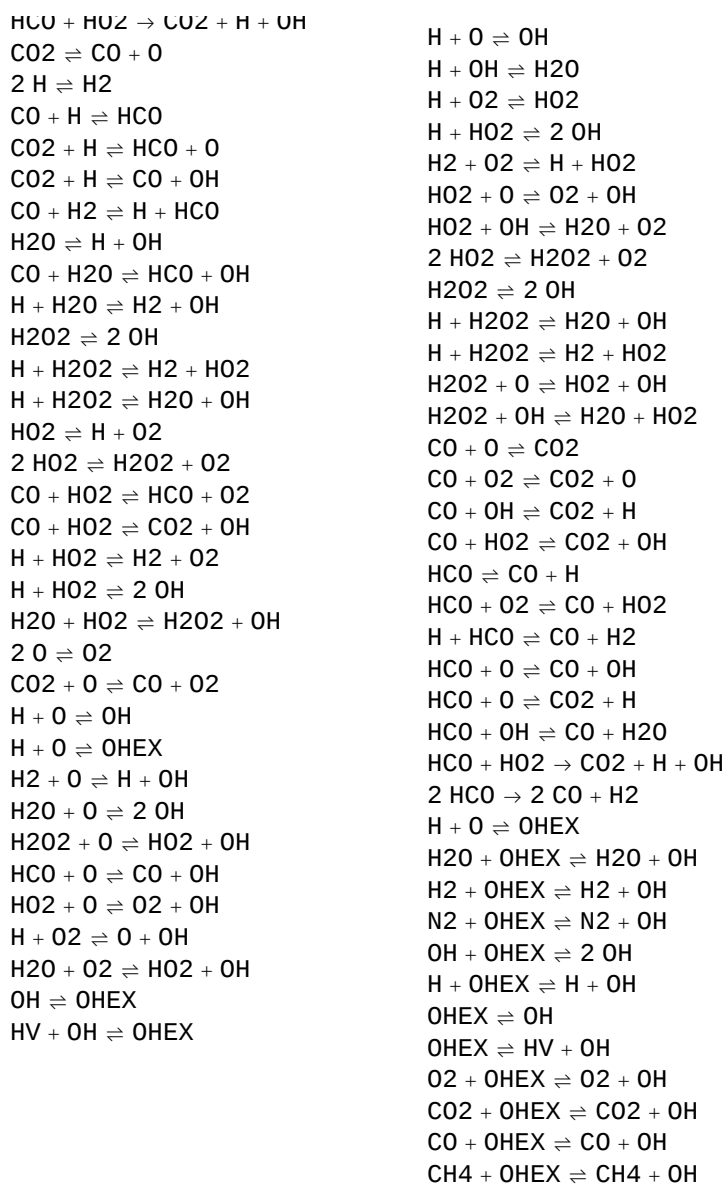
Orig. Mechanism



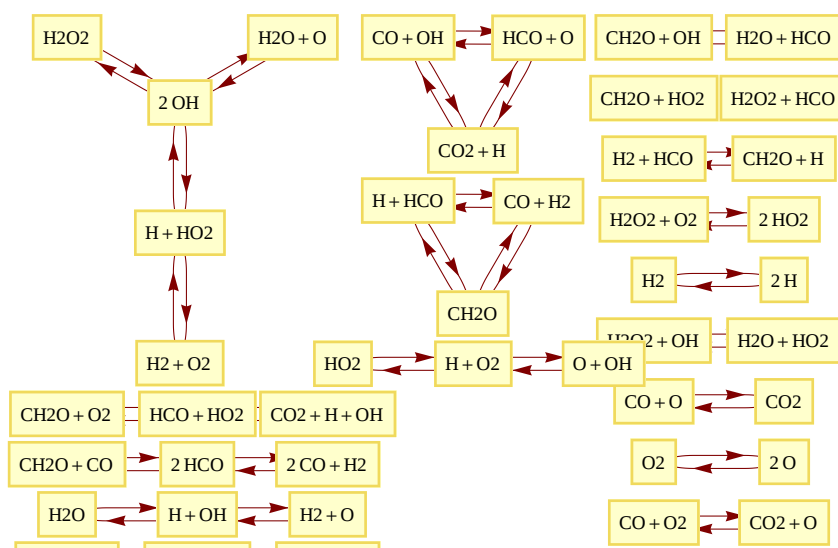
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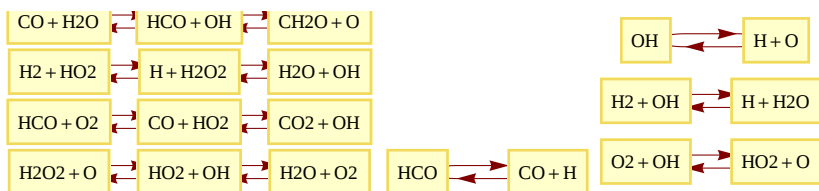


HCO + HCO → CO + CO + H2

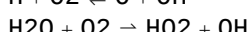
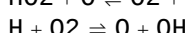
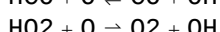
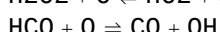
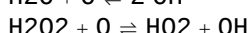
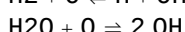
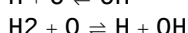
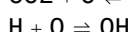
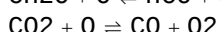
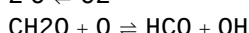
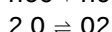
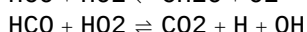
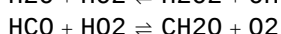
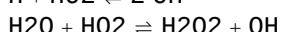
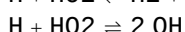
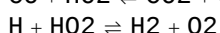
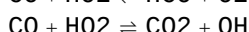
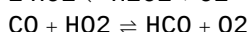
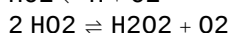
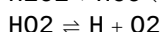
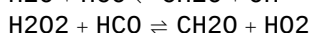
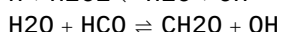
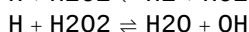
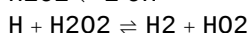
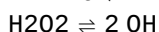
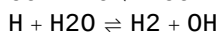
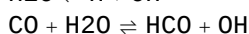
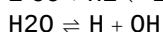
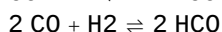
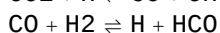
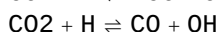
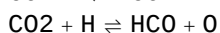
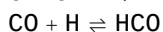
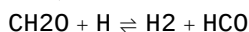
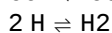
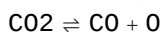
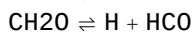
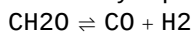


Li2007

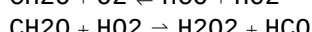
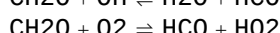
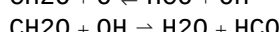
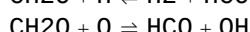
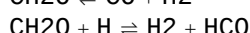
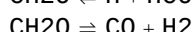
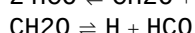
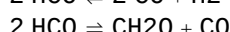
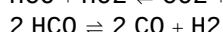
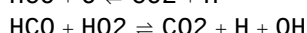
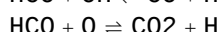
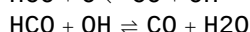
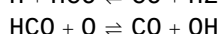
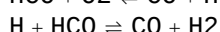
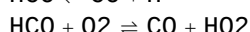
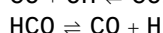
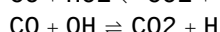
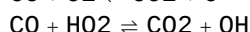
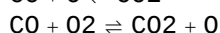
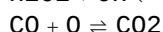
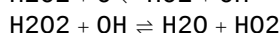
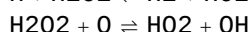
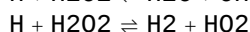
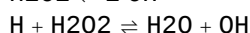
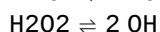
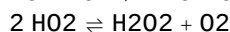
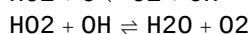
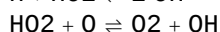
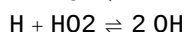
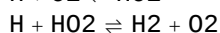
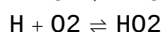
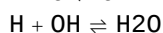
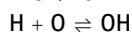
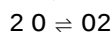
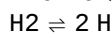
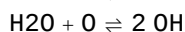
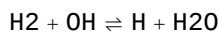
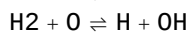
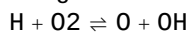




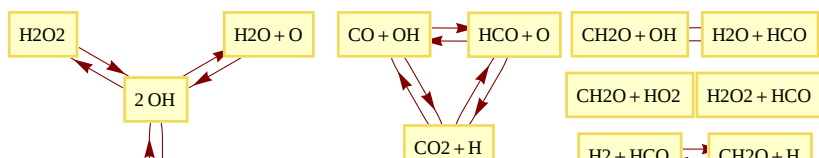
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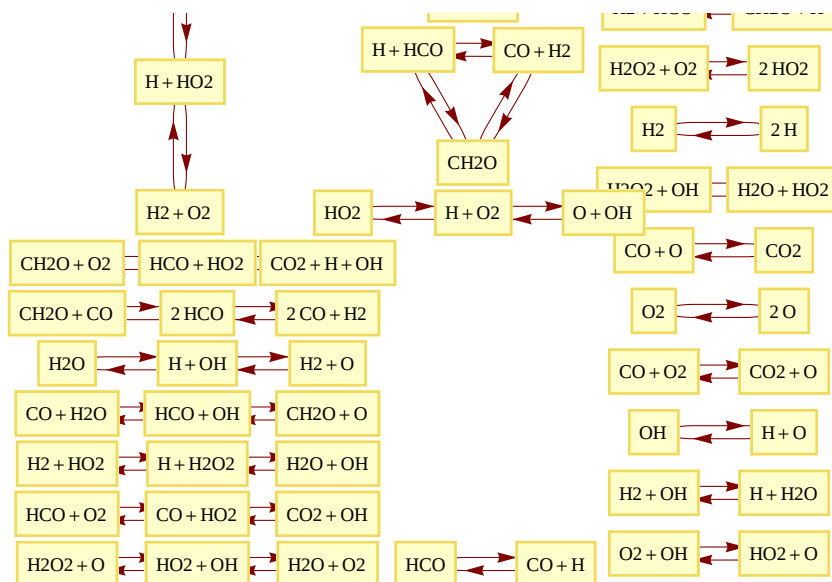


Orig. Mechanism

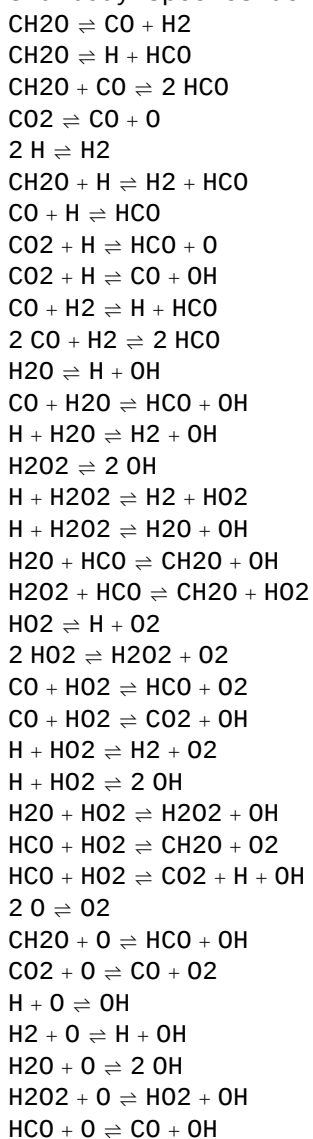


NUIG2010

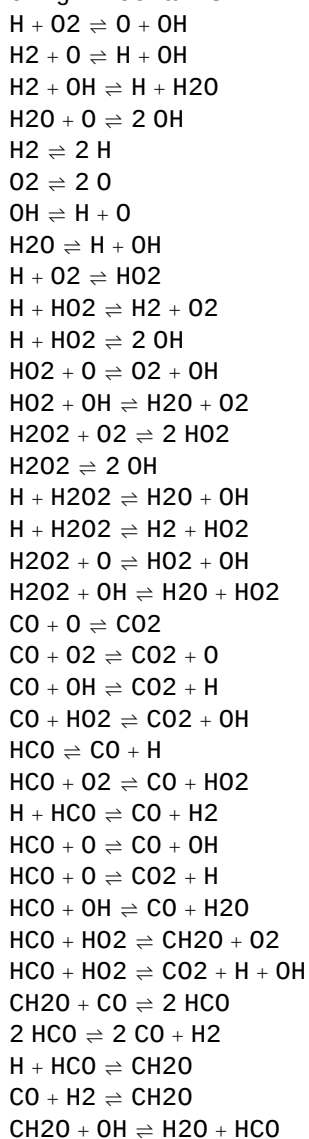


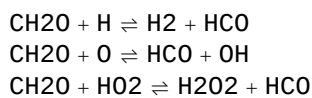
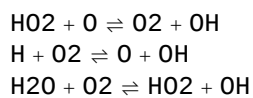


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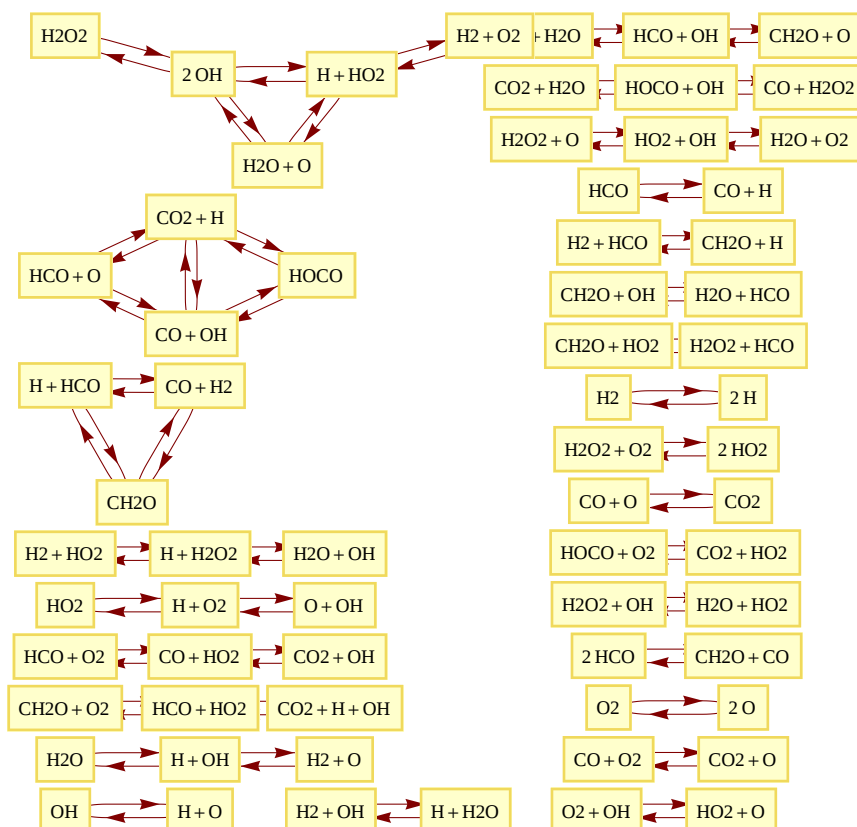


Orig. Mechanism

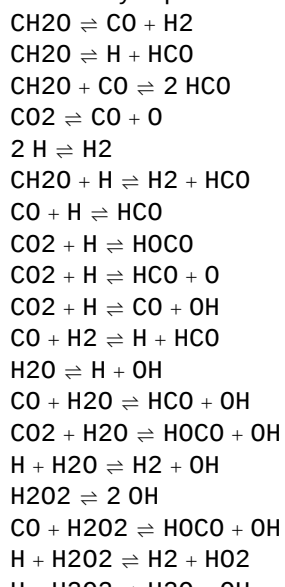




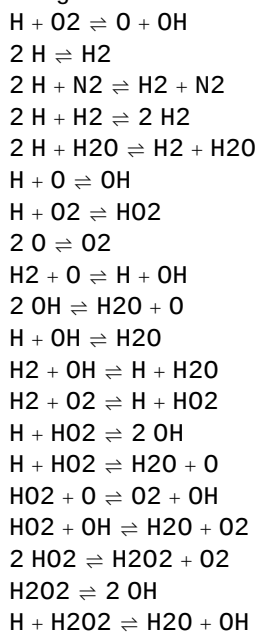
Rasmussen2008

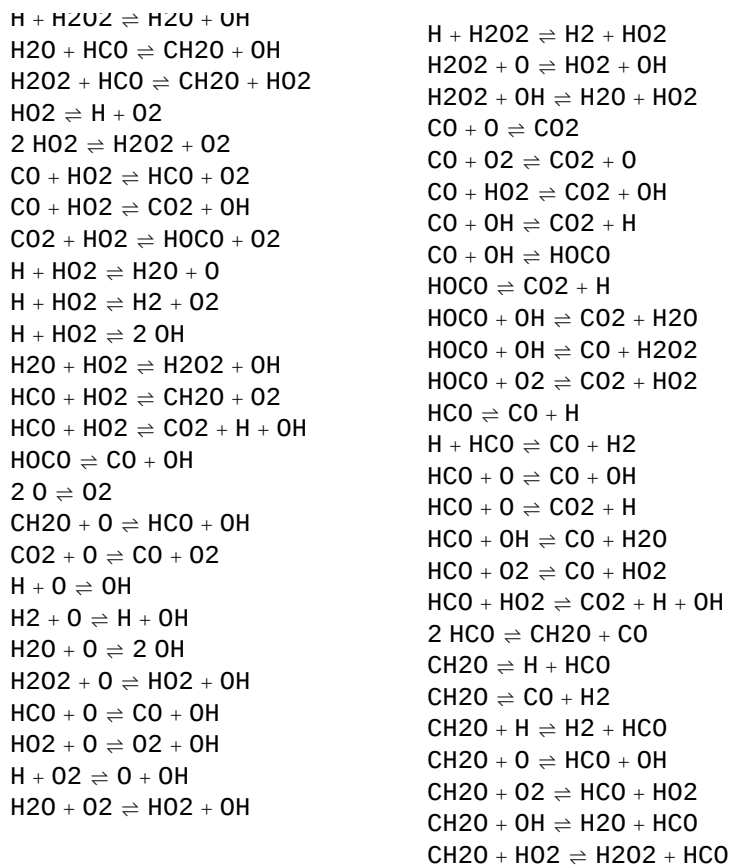


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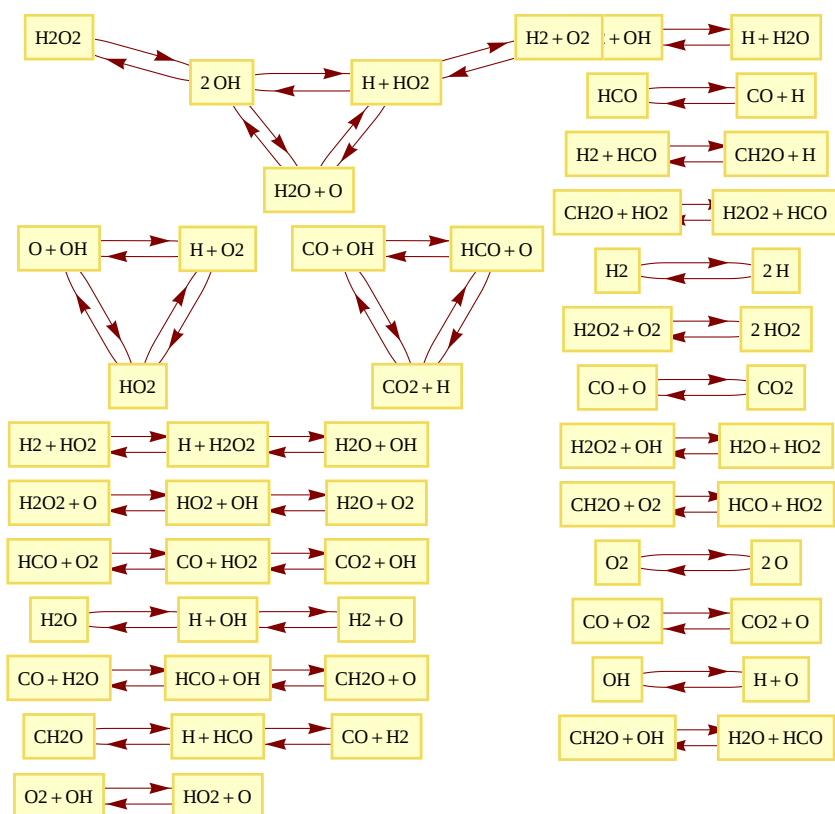


Orig. Mechanism



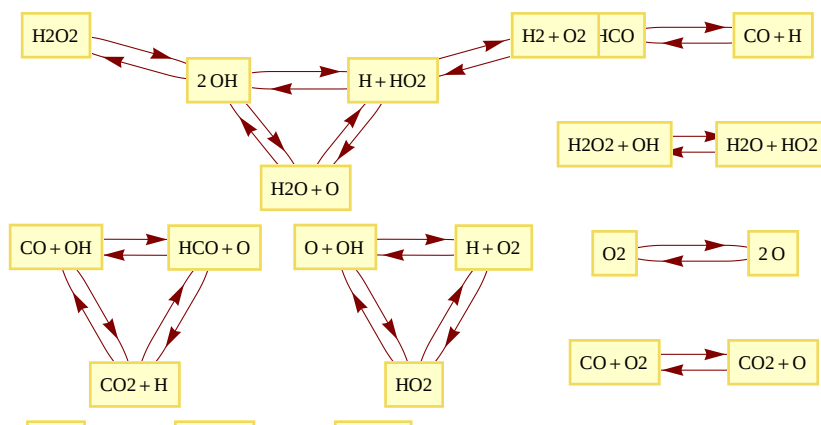


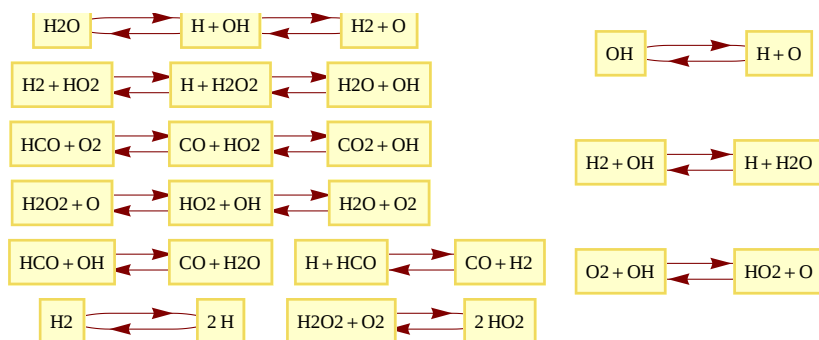
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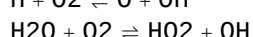
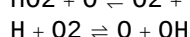
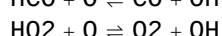
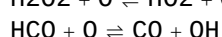
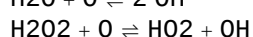
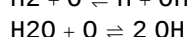
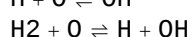
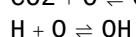
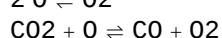
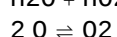
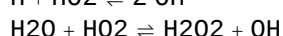
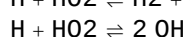
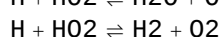
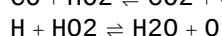
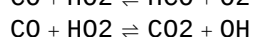
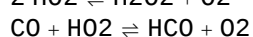
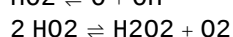
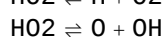
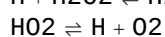
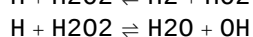
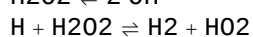
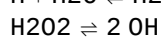
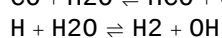
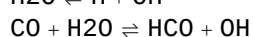
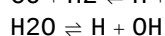
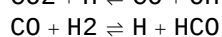
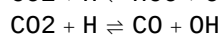
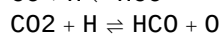
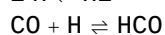
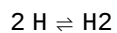
3rd body species deleted	Orig. Mechanism
$\text{CH}_2\text{O} \rightleftharpoons \text{H} + \text{HCO}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$
$\text{CO}_2 \rightleftharpoons \text{CO} + \text{O}$	$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$
$2 \text{H} \rightleftharpoons \text{H}_2$	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$
$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{H}_2 + \text{HCO}$	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2 \text{OH}$
$\text{CO} + \text{H} \rightleftharpoons \text{HCO}$	$2 \text{H} \rightleftharpoons \text{H}_2$
$\text{CO}_2 + \text{H} \rightleftharpoons \text{HCO} + \text{O}$	$\text{H} + \text{OH} \rightleftharpoons \text{H}_2\text{O}$
$\text{CO}_2 + \text{H} \rightleftharpoons \text{CO} + \text{OH}$	$2 \text{O} \rightleftharpoons \text{O}_2$
$\text{CO} + \text{H}_2 \rightleftharpoons \text{H} + \text{HCO}$	$\text{H} + \text{O} \rightleftharpoons \text{OH}$
$\text{H}_2\text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{O} + \text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{HCO} + \text{OH}$	$\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2$
$\text{H} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \text{OH}$	$\text{H} + \text{HO}_2 \rightleftharpoons 2 \text{OH}$
$\text{H}_2\text{O}_2 \rightleftharpoons 2 \text{OH}$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2 + \text{O}_2$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$	$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$
$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$
$\text{H}_2\text{O} + \text{HCO} \rightleftharpoons \text{CH}_2\text{O} + \text{OH}$	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
$\text{H}_2\text{O}_2 + \text{HCO} \rightleftharpoons \text{CH}_2\text{O} + \text{HO}_2$	$2 \text{OH} \rightleftharpoons \text{H}_2\text{O}_2$
$\text{HO}_2 \rightleftharpoons \text{H} + \text{O}_2$	$2 \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$
$\text{HO}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2 + \text{HO}_2$
$2 \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	$\text{H} + \text{H}_2\text{O}_2 \rightleftharpoons \text{H}_2\text{O} + \text{OH}$
$\text{CO} + \text{HO}_2 \rightleftharpoons \text{HCO} + \text{O}_2$	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$
$\text{CO} + \text{HO}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$
$\text{H} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$\text{CO} + \text{O} \rightleftharpoons \text{CO}_2$
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$\text{H} + \text{HO}_2 \rightleftharpoons 2 \text{OH}$	$\text{CO} + \text{HO}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$
$\text{H}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{CO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{O}$
$\text{HCO} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{O}_2$	$\text{HCO} \rightleftharpoons \text{CO} + \text{H}$
$2 \text{O} \rightleftharpoons \text{O}_2$	$\text{H} + \text{HCO} \rightleftharpoons \text{CO} + \text{H}_2$
$\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{HCO} + \text{OH}$	$\text{HCO} + \text{O} \rightleftharpoons \text{CO} + \text{OH}$
$\text{CO}_2 + \text{O} \rightleftharpoons \text{CO} + \text{O}_2$	$\text{HCO} + \text{O} \rightleftharpoons \text{CO}_2 + \text{H}$
$\text{H} + \text{O} \rightleftharpoons \text{OH}$	$\text{HCO} + \text{OH} \rightleftharpoons \text{CO} + \text{H}_2\text{O}$
$\text{H}_2 + \text{O} \rightleftharpoons \text{H} + \text{OH}$	$\text{HCO} + \text{O}_2 \rightleftharpoons \text{CO} + \text{HO}_2$
$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2 \text{OH}$	$\text{H} + \text{HCO} \rightleftharpoons \text{CH}_2\text{O}$
$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$	$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{H}_2 + \text{HCO}$
$\text{HCO} + \text{O} \rightleftharpoons \text{CO} + \text{OH}$	$\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{HCO} + \text{OH}$
$\text{HO}_2 + \text{O} \rightleftharpoons \text{O}_2 + \text{OH}$	$\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HCO}$
$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	$\text{CH}_2\text{O} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{HO}_2$
$\text{H}_2\text{O} + \text{O}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{OH}$	$\text{CH}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{HCO}$

SaxenaWilliams2006

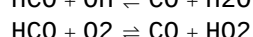
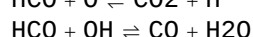
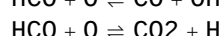
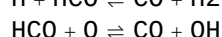
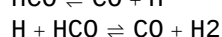
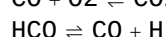
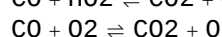
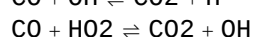
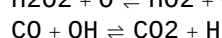
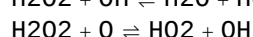
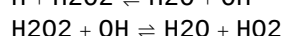
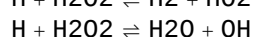
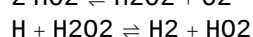
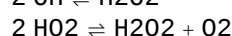
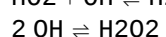
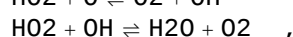
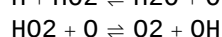
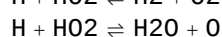
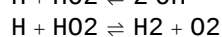
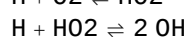
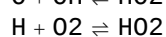
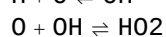
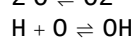
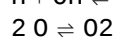
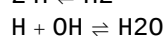
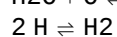
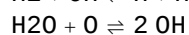
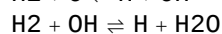
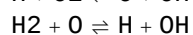
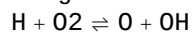




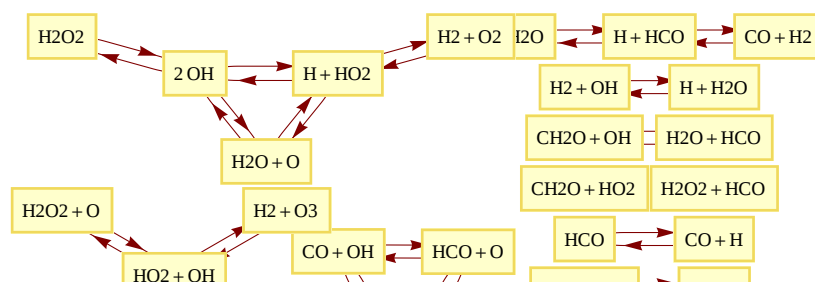
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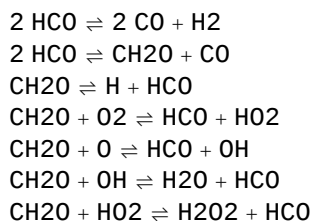
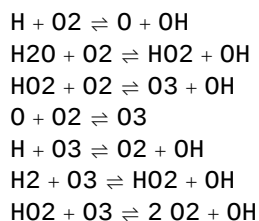


Orig. Mechanism

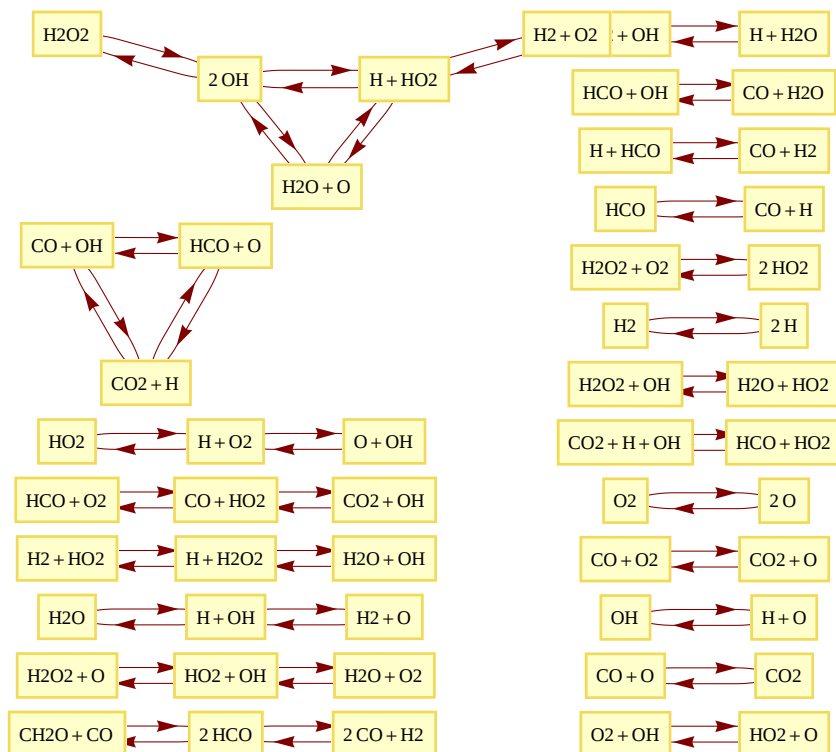


Starik2009

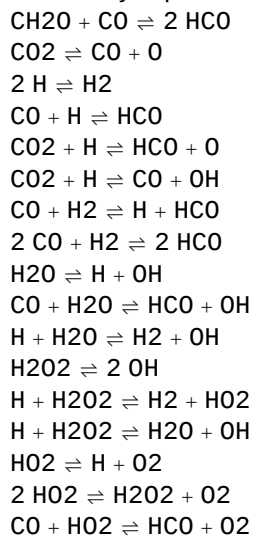




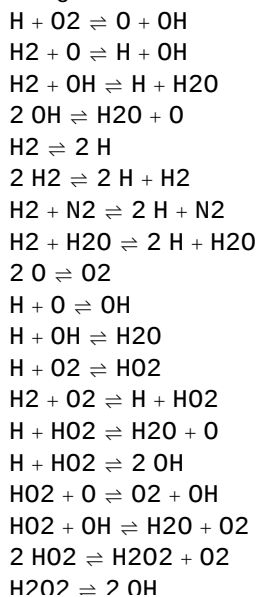
Sun2007

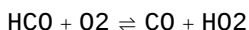
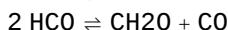
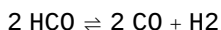
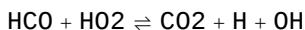
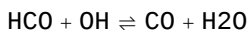
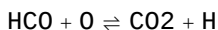
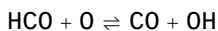
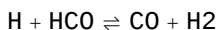
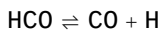
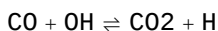
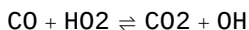
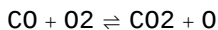
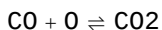
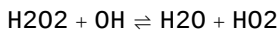
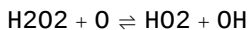
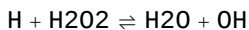
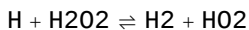
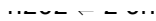
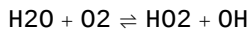
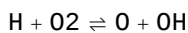
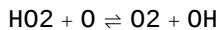
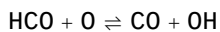
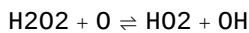
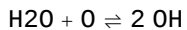
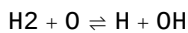
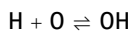
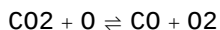
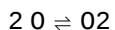
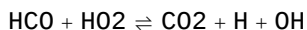
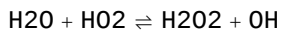
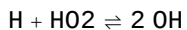
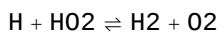
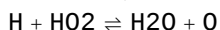
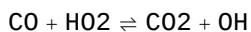


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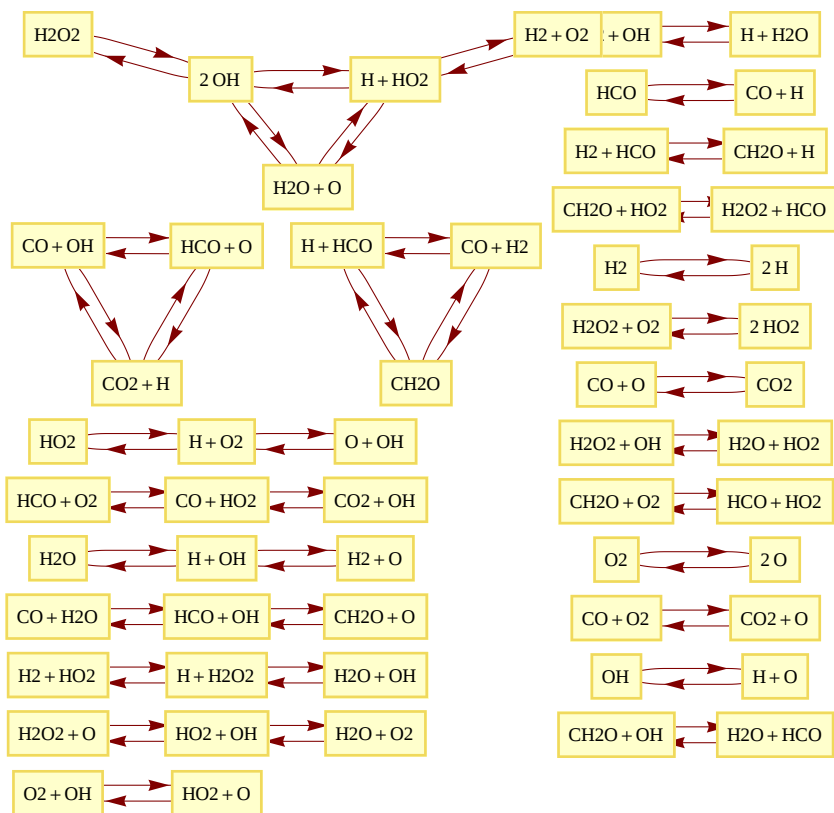


Orig. Mechanism

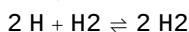
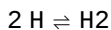
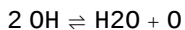
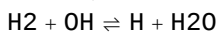
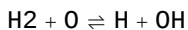
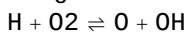




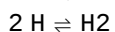
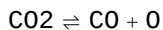
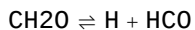
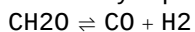
USC2007

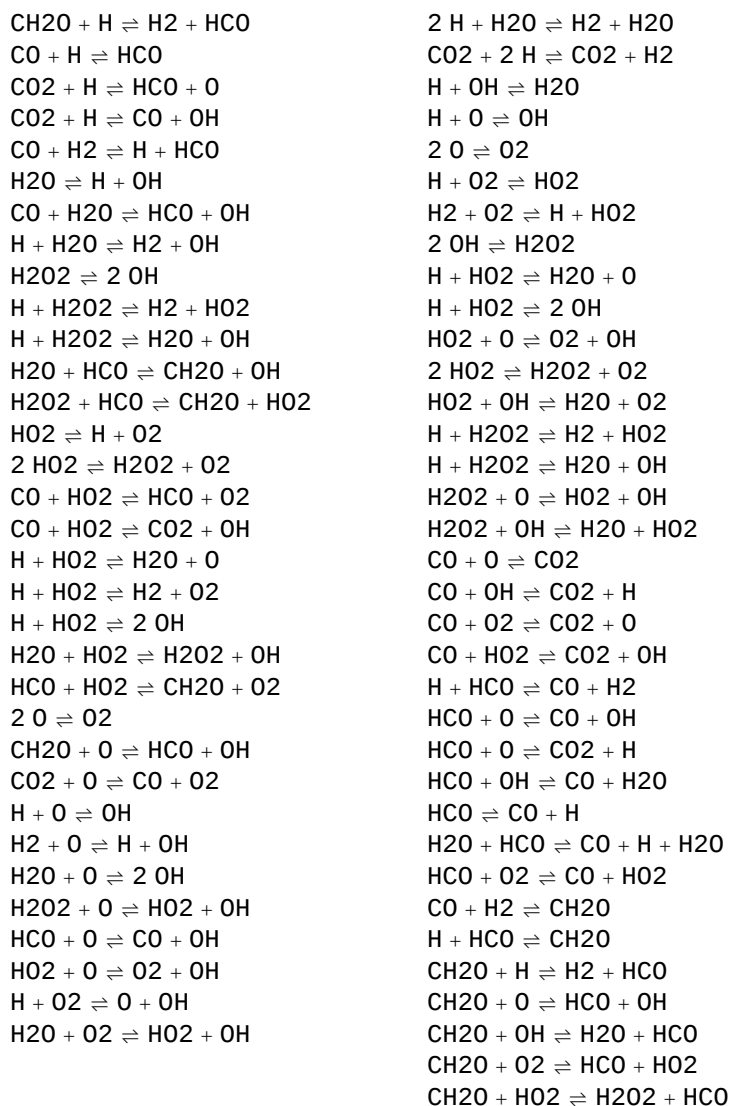


Orig. Mechanism

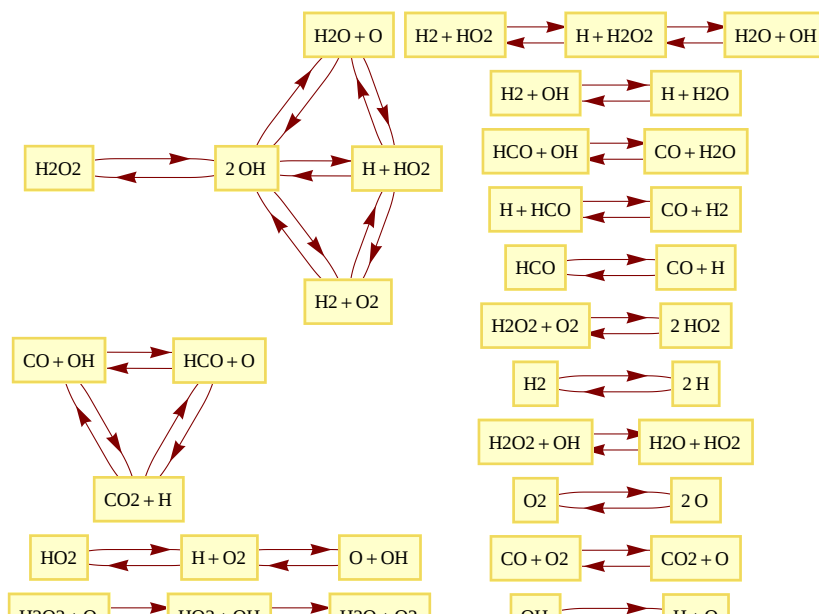


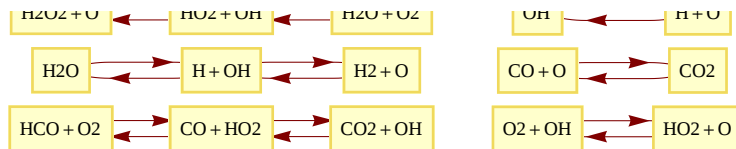
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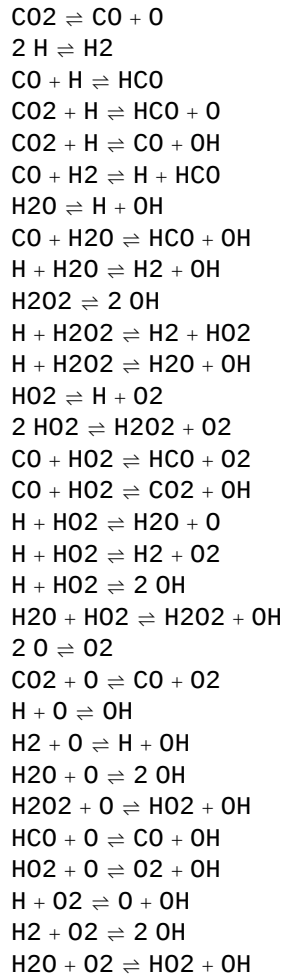


Zsely2005

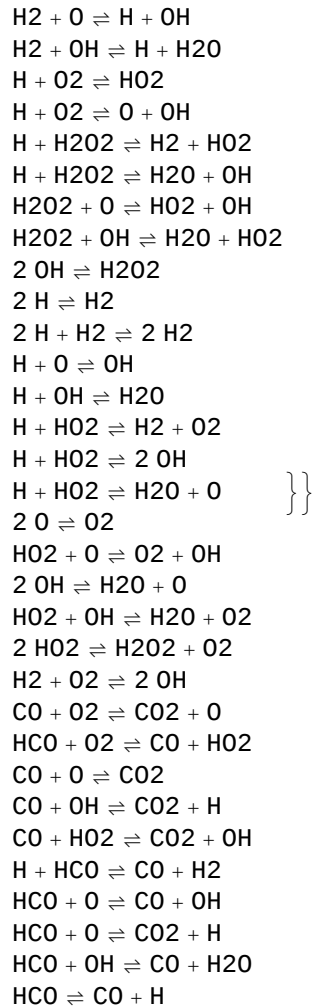




3rd body species deleted



Orig. Mechanism



Show Less

Show More

Show Full Output

Set Size Limit...

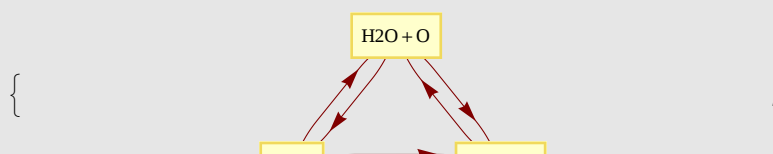
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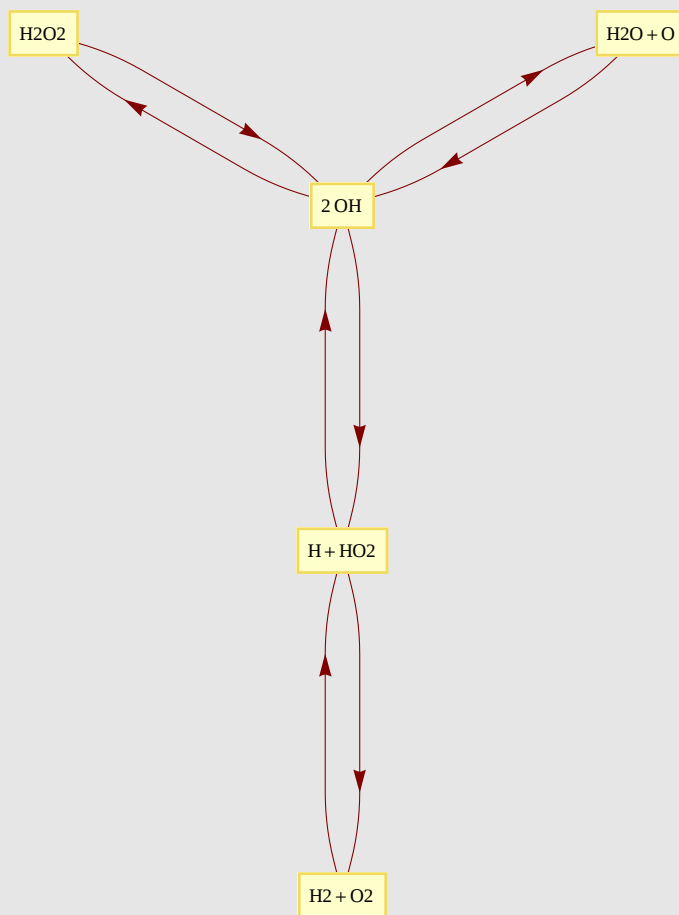
maxfhjedges = Flatten[(First /@ #) & /@ maxfhjcomponents, 1];

GraphPlot[First[#], VertexLabeling → True, DirectedEdges → True,
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ToString[coevery[Last[#], 3]] <> "\n"] & /@
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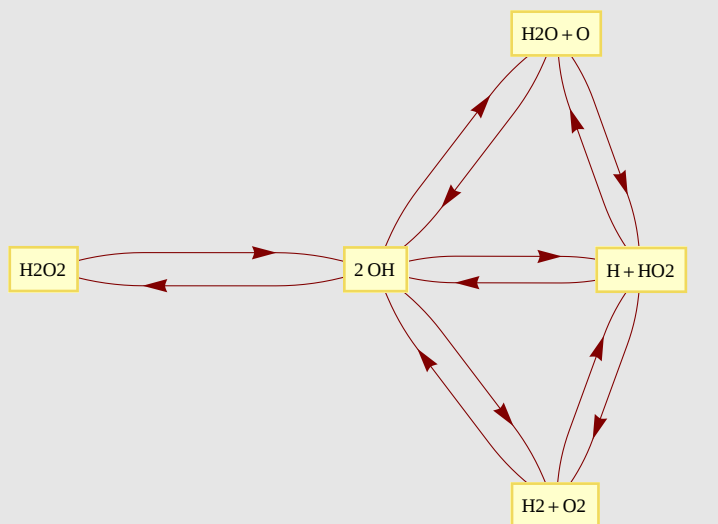
Max weakly connected component of mech Ahmed2007



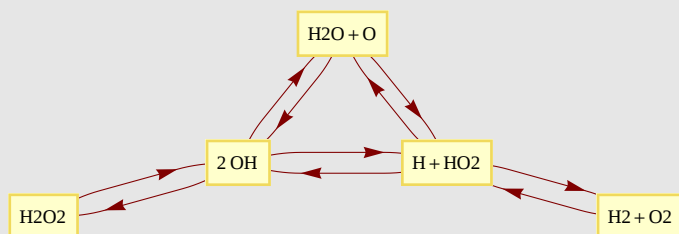
Max weakly connected component of mech CRECK2012



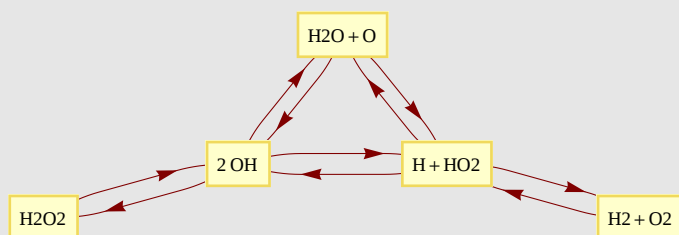
Max weakly connected component of mech Dagaut2003



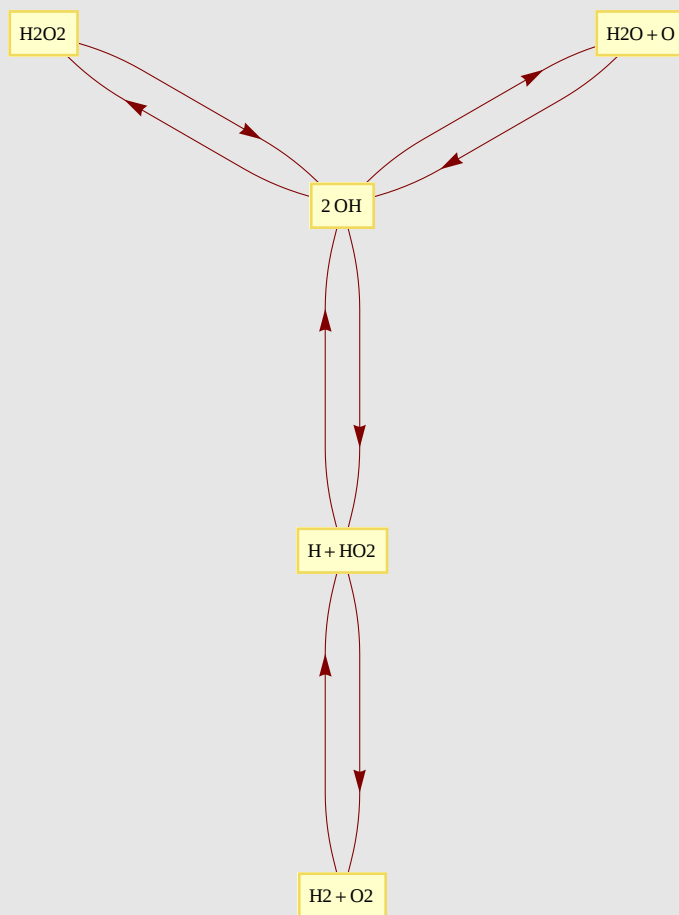
Max weakly connected component of mech Davis2005



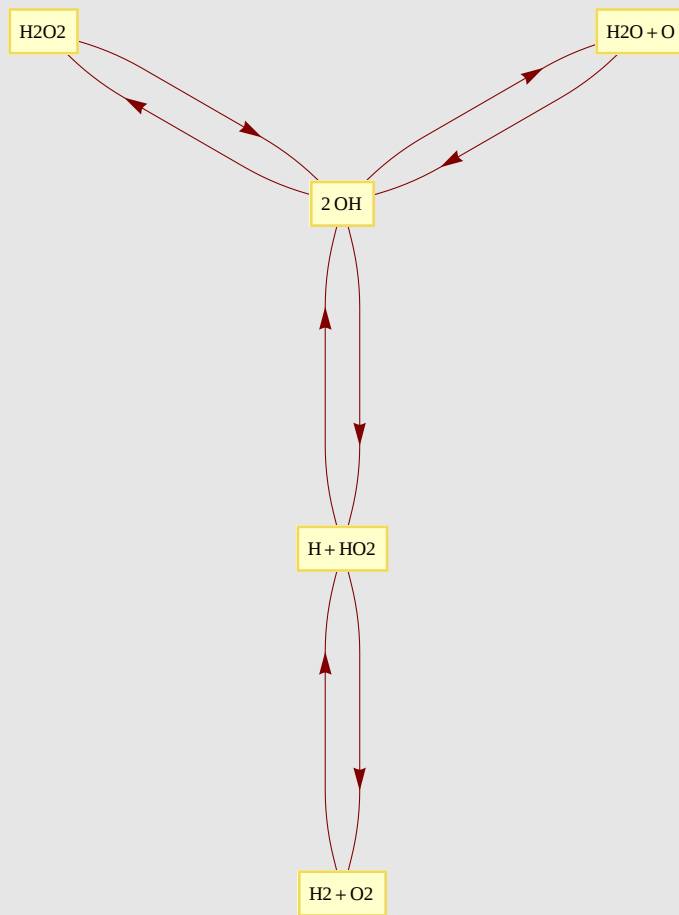
Max weakly connected component of mech gri30



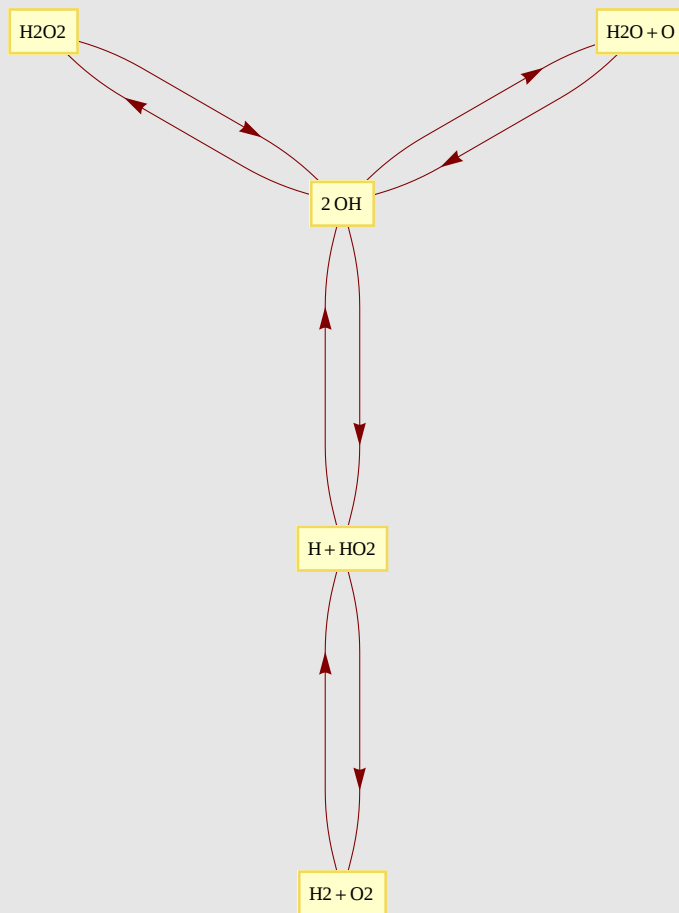
Max weakly connected component of mech Keromnes2013



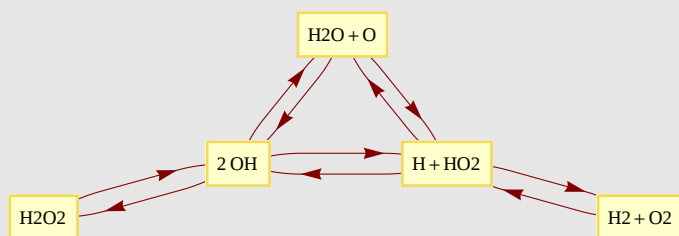
Max weakly connected component of mech Li2007



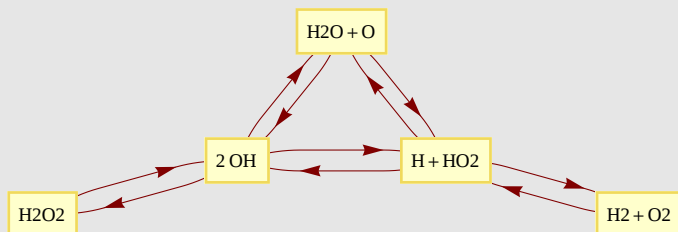
Max weakly connected component of mech NUIG2010



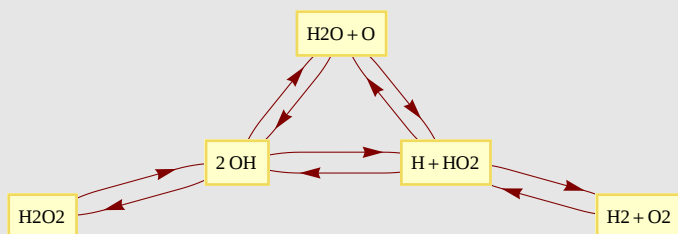
Max weakly connected component of mech Rasmussen2008



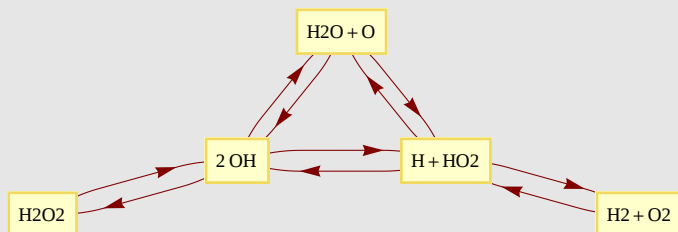
Max weakly connected component of mech SanDiego2011



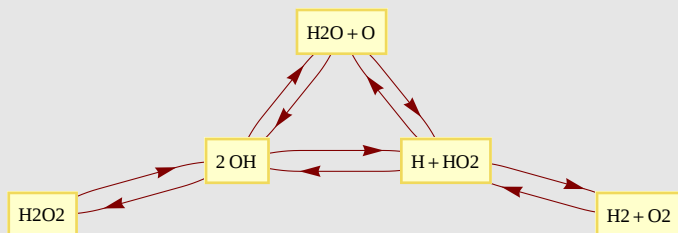
Max weakly connected component of mech SaxenaWilliams2006



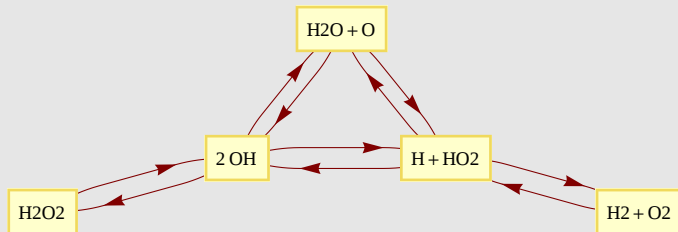
Max weakly connected component of mech Starik2009



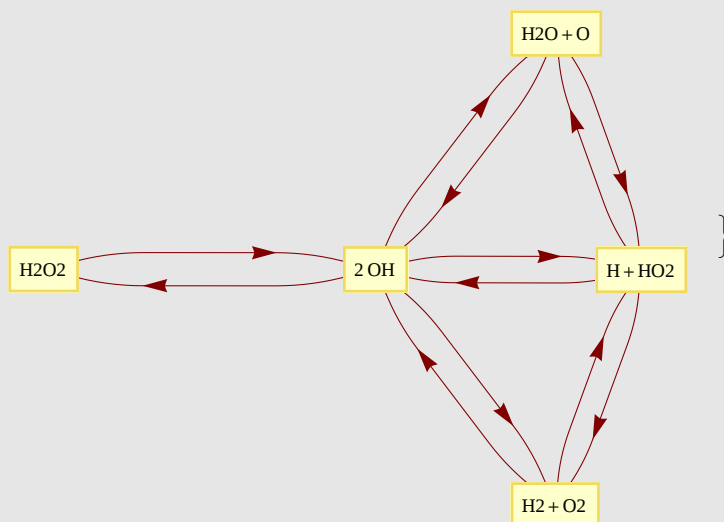
Max weakly connected component of mech Sun2007



Max weakly connected component of mech USC2007



Max weakly connected component of mech Zsely2005



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	Ahmed2007	CRECK2012	Dagaut2003	Davis2005	gri30
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CRECK2012	False	TRUE	False	False	False
Dagaut2003	False	False	TRUE	False	False
Davis2005	False	False	False	TRUE	False
gri30	False	False	False	False	TRUE
Keromnes2013	False	False	False	False	False
Li2007	False	False	False	False	False
NUIG2010	False	False	False	False	False
Rasmussen2008	False	False	False	False	False
SanDiego2011	False	False	False	False	False
SaxenaWilliams2006	False	False	False	False	False
Starik2009	False	False	False	False	False
Sun2007	False	False	False	False	False
USC2007	False	False	False	False	TRUE
Zsely2005	False	False	False	False	False

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12	F	F	F	F	F	F	F	F	F	F	F	T	F	F	F
13	F	F	F	F	F	F	F	F	F	F	F	F	T	F	F
14	F	F	F	F	T	F	F	F	F	F	F	F	F	T	F
15	F	F	F	F	F	F	F	F	F	F	F	F	F	F	T

```
ag = (tt /. {Style["TRUE", Bold] → 1, False → 0}) - IdentityMatrix[15];
```

```
AdjacencyGraph[ag, ImageSize → 1000, ImagePadding → 50, VertexLabels →
  Thread[Rule[indices, Style[#, Bold, 12] & /@ coevery[[indices, 3]]]]]
```



```
wc = ConnectedComponents[AdjacencyGraph[ag]] /.
  Thread[Rule[indices, coevery[[indices, 3]]]];
```

```
TableForm[wc, TableHeadings → {Range[13], None}]
```

1	Ahmed2007	
2	CRECK2012	
3	Dagaut2003	
4	Davis2005	
5	gri30	USC2007
6	Keromnes2013	
7	Li2007	NUIG2010
8	Rasmussen2008	
9	SanDiego2011	
10	SaxenaWilliams2006	
11	Starik2009	
12	Sun2007	
13	Zsely2005	

```
reducedindices = Sort[First /@ ConnectedComponents[AdjacencyGraph[ag]]]
```

```
{1, 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 15}
```

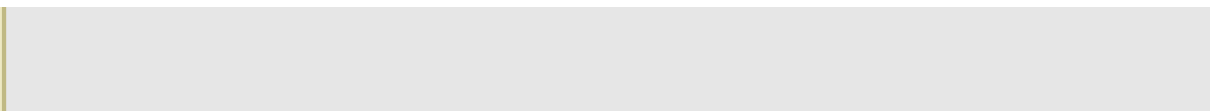
```
Column[
```

```
  Riffle[Row /@ (Join[{Style[coevery[[#, 3]], Bold, 14], "\t"}, VolpertIndexing[
    coevery[[#, 2]], {"H2", "O2", "CO"}, Verbose → True,
    ExternalSpecies → {"HV"}}] & /@ reducedindices), "\n\n"], 2]
```

		Reaction steps	Indices
		CO + O2 → CO2 + O	0
		O2 → 2 O	0
		H2 + O2 → H + HO2	0
		CO + H2 → H + HCO	0
		H2 → 2 H	0
		H + O2 → O + OH	1
		HO2 + O → O2 + OH	1
		HCO + O → CO + OH	1
		H2 + O → H + OH	1
		CO2 + O → CO + O2	1
		2 O → O2	1
		HCO + HO2 → CH2O + O2	1
		H + HO2 → 2 OH	1
		H + HO2 → H2 + O2	1
		H + HO2 → H2O + O	1
		CO + HO2 → CO2 + OH	1
		HCO + O2 → CO + HO2	1
		CO + HO2 → HCO + O2	1
		2 HO2 → H2O2 + O2	1
		H + O2 → HO2	1
		HO2 → H + O2	1
		H2 + HO2 → H + H2O2	1
		H + HCO → CO + H2	1
		CO2 + H → CO + OH	1
		HCO + O → CO2 + H	1
		CO2 + H → HCO + O	1
		HCO → CO + H	1
		CO + H → HCO	1
		H2 + HCO → CH2O + H	1
		2 H → H2	1
		CO + O → CO2	1
		CO2 → CO + O	1
		2 HCO → CH2O + CO	1
		H + HCO → CH2O	1
		HO2 + OH → H2O + O2	2
		H2O + O2 → HO2 + OH	2

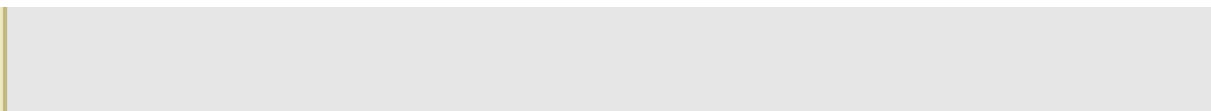
Species	Indices
O2	0
H2	0
CO	0
HO2	1
O	1
CO2	1

Ahmed2007



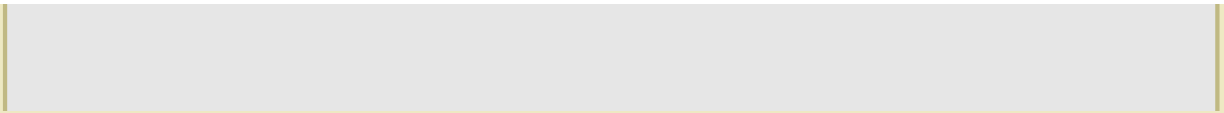
CRECK2012

		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{HO}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CO} + \text{H}_2\text{O}_2$	1
		$\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{O} + \text{OH} \rightarrow \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2
		$\text{CO} + \text{H}_2\text{O}_2 \rightarrow \text{HCO} + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$	2
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2



Dagaut2003

		Reaction steps	Indices
		$\text{H}_2 + \text{O}_2 \rightarrow 2 \text{OH}$	0
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	0
		$2 \text{CO} + \text{H}_2 \rightarrow 2 \text{HCO}$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	1
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{OH} \rightarrow \text{H} + \text{O}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{CO}_2 + \text{H} + \text{OH} \rightarrow \text{HCO} + \text{H}_2\text{O}_2$	1
		$\text{HCO} + \text{H}_2\text{O}_2 \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
		$2 \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}_2$	1
		$\text{CO} + \text{H}_2\text{O}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}_2$	1
		$\text{CO} + \text{H}_2\text{O}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2\text{O}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	1
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	1
		$2 \text{HCO} \rightarrow 2 \text{CO} + \text{H}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$2 \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{CO}$	1
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2



Davis2005

		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO} + \text{H}_2\text{O}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}_2$	1
		$\text{CO} + \text{H}_2\text{O}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2\text{O}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O}_2$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	2

Species

Indices

O2

0

H2

0

CO

0

H2O2

1

HCO

1

H

1

O

1

CO2

1

H2O2

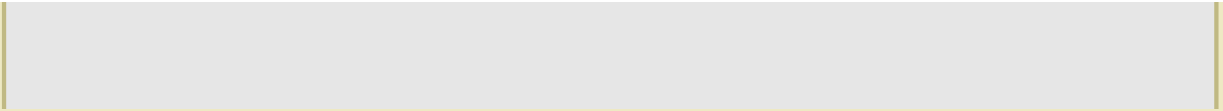
2

H2O

2

OH

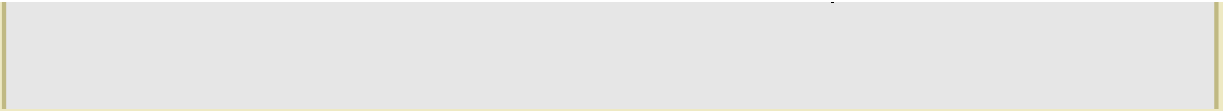
2



gri30

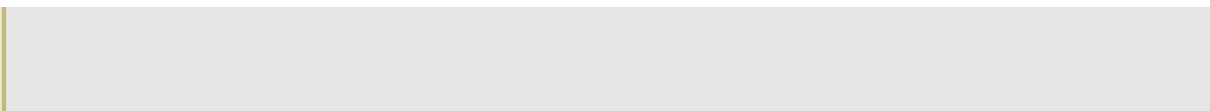
Species	Indices
O2	0
H2	0
CO	0
H2O2	1
O	1
CO2	1
HCO	1
H	1
CH2O	1
H2O2	2
H2O	2
OH	2

Reaction steps	Indices
CO + O2 → CO2 + O	0
O2 → 2 O	0
H2 + O2 → H + H2O2	0
CO + H2 → H + HCO	0
H2 → 2 H	0
CO + H2 → CH2O	0
H + O2 → O + OH	1
H2O2 + O → O2 + OH	1
HCO + O → CO + OH	1
H2 + O → H + OH	1
H + O → OH	1
CO2 + O → CO + O2	1
CH2O + O → HCO + OH	1
2 O → O2	1
CH2O + O2 → HCO + H2O2	1
HCO + H2O2 → CH2O + O2	1
H + H2O2 → 2 OH	1
H + H2O2 → H2 + O2	1
H + H2O2 → H2O + O	1
CO + H2O2 → CO2 + OH	1
HCO + O2 → CO + H2O2	1
CO + H2O2 → HCO + O2	1
2 H2O2 → H2O2 + O2	1
H + O2 → H2O2	1
H2O2 → H + O2	1
CH2O + H2O2 → H2O2 + HCO	1
H2 + H2O2 → H + H2O2	1
H + HCO → CO + H2	1
CO2 + H → CO + OH	1
HCO + O → CO2 + H	1
CO2 + H → HCO + O	1
HCO → CO + H	1
CO + H → HCO	1
H2 + HCO → CH2O + H	1
CH2O + H → H2 + HCO	1
2 H → H2	1
CO + O → CO2	1
CO2 → CO + O	1
H + HCO → CH2O	1
CH2O → H + HCO	1
CH2O → CO + H2	1
H2O2 + OH → H2O + O2	2
H2O + O2 → H2O2 + OH	2
O + OH → H + O2	2
O2 + OH → H2O2 + O	2
CO + OH → HCO + O	2
H2O2 + OH → H2O2 + O	2
H2O2 + O → H2O2 + OH	2
2 OH → H2O + O	2
H2O + O → 2 OH	2
H + OH → H2 + O	2
OH → H + O	2
HCO + OH → CH2O + O	2
H2O2 + OH → H2O + H2O2	2
H2O + H2O2 → H2O2 + OH	2
2 OH → H + H2O2	2
H2O + O → H + H2O2	2
CO2 + OH → CO + H2O2	2
H2O2 + O2 → 2 H2O2	2
H2O2 + HCO → CH2O + H2O2	2
CH2O + OH → H2O + HCO	2
H2O + HCO → CH2O + OH	2
H2O + OH → H + H2O2	2
H + H2O2 → H2O + OH	2



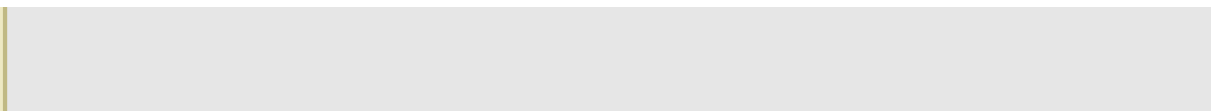
Keromnes2013

		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OHEX}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
		$2 \text{HCO} \rightarrow 2 \text{CO} + \text{H}_2$	1
		$\text{OHEX} \rightarrow \text{OH}$	2
		$\text{OH} \rightarrow \text{OHEX}$	2
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OHEX} \rightarrow \text{H} + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{OH}$	3
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	3
		$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	3
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	3
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	3
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{OH}$	3
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	3



Li2007

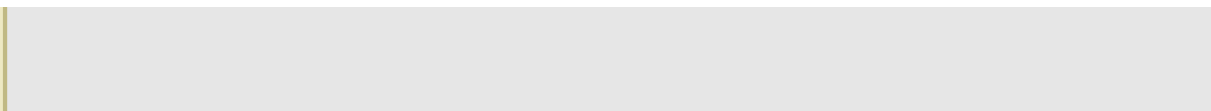
		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$2 \text{CO} + \text{H}_2 \rightarrow 2 \text{HCO}$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{CH}_2\text{O}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$\text{CH}_2\text{O} + \text{O} \rightarrow \text{HCO} + \text{OH}$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
		$\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{HCO} + \text{HO}_2$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CH}_2\text{O} + \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{HCO}$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2 \text{HCO} \rightarrow 2 \text{CO} + \text{H}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$\text{H}_2 + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{H}$	1
		$\text{CH}_2\text{O} + \text{H} \rightarrow \text{H}_2 + \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$2 \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{CO}$	1
		$\text{CH}_2\text{O} + \text{CO} \rightarrow 2 \text{HCO}$	1
		$\text{H} + \text{HCO} \rightarrow \text{CH}_2\text{O}$	1
		$\text{CH}_2\text{O} \rightarrow \text{H} + \text{HCO}$	1
		$\text{CH}_2\text{O} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{O}$	2
		$\text{CO}_2 + \text{H} + \text{OH} \rightarrow \text{HCO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	2
		$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCO}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2



Rasmussen2008

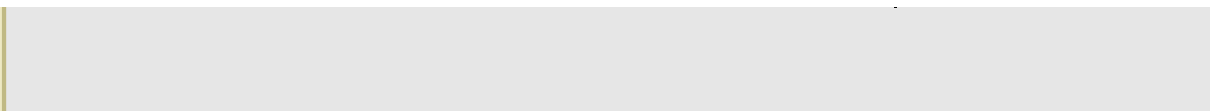
Species	Indices
O2	0
H2	0
CO	0
H2O	1
O	1
CO2	1
HCO	1
H	1
CH2O	1
H2O2	2
H2O	2
OH	2
HOCO	2

Reaction steps	Indices
$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
$\text{O}_2 \rightarrow 2 \text{O}$	0
$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}$	0
$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
$\text{H}_2 \rightarrow 2 \text{H}$	0
$\text{CO} + \text{H}_2 \rightarrow \text{CH}_2\text{O}$	0
$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
$\text{H}_2\text{O} + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
$\text{H} + \text{O} \rightarrow \text{OH}$	1
$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
$\text{CH}_2\text{O} + \text{O} \rightarrow \text{HCO} + \text{OH}$	1
$2 \text{O} \rightarrow \text{O}_2$	1
$\text{HCO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
$\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{HCO} + \text{H}_2\text{O}$	1
$\text{HCO} + \text{H}_2\text{O} \rightarrow \text{CH}_2\text{O} + \text{O}_2$	1
$\text{H} + \text{H}_2\text{O} \rightarrow 2 \text{OH}$	1
$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}_2$	1
$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{O}$	1
$\text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{HOCO} + \text{O}_2$	1
$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{OH}$	1
$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	1
$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{O}_2$	1
$2 \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}$	1
$\text{H}_2\text{O} \rightarrow \text{H} + \text{O}_2$	1
$\text{CH}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{HCO}$	1
$\text{H}_2 + \text{H}_2\text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
$\text{CO}_2 + \text{H} \rightarrow \text{HOCO}$	1
$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
$\text{H}_2 + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{H}$	1
$\text{CH}_2\text{O} + \text{H} \rightarrow \text{H}_2 + \text{HCO}$	1
$2 \text{H} \rightarrow \text{H}_2$	1
$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
$2 \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{CO}$	1
$\text{CH}_2\text{O} + \text{CO} \rightarrow 2 \text{HCO}$	1
$\text{H} + \text{HCO} \rightarrow \text{CH}_2\text{O}$	1
$\text{CH}_2\text{O} \rightarrow \text{H} + \text{HCO}$	1
$\text{CH}_2\text{O} \rightarrow \text{CO} + \text{H}_2$	1
$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O} + \text{OH}$	2
$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
$\text{OH} \rightarrow \text{H} + \text{O}$	2
$\text{HCO} + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{O}$	2
$\text{CO} + \text{OH} \rightarrow \text{HOCO}$	2
$\text{HOCO} \rightarrow \text{CO} + \text{OH}$	2
$\text{CO}_2 + \text{H} + \text{OH} \rightarrow \text{HCO} + \text{H}_2\text{O}$	2
$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	2
$\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
$2 \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2



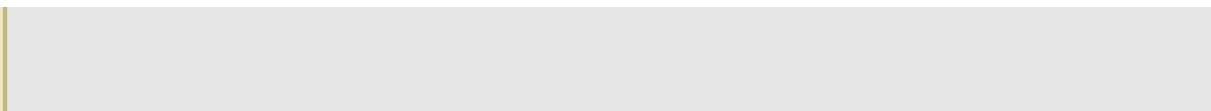
SanDiego2011

		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CH}_2\text{O} + \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{HO}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$\text{H}_2 + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{H}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$\text{H} + \text{HCO} \rightarrow \text{CH}_2\text{O}$	1
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{O}$	2
		$\text{CH}_2\text{O} + \text{O} \rightarrow \text{HCO} + \text{OH}$	2
		$\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{HCO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{O} + \text{OH} \rightarrow \text{HO}_2$	2
		$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{HCO}$	2
		$\text{H}_2\text{O}_2 + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	2
		$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCO}$	2
		$\text{H}_2\text{O} + \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{OH}$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2



SaxenaWilliams2006

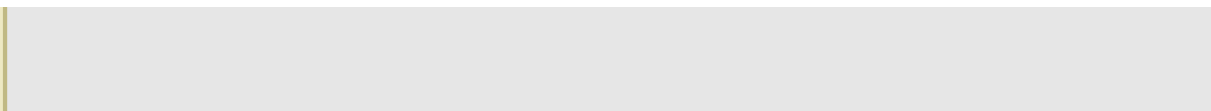
		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{H}_2\text{O}$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O} \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	1
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H}_2\text{O} \rightarrow \text{O} + \text{OH}$	1
		$\text{H} + \text{O}_2 \rightarrow \text{H}_2\text{O}$	1
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{H}_2\text{O} \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}$	2
		$\text{O} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	2



Starik2009

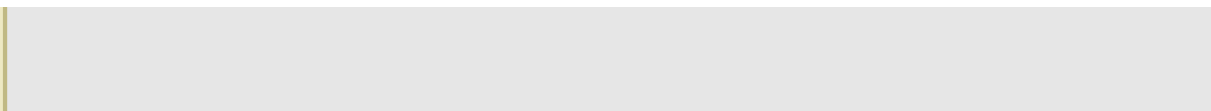
Species	Indices
O2	0
H2	0
CO	0
O3	1
H02	1
O	1
CO2	1
HCO	1
H	1
H2O2	2
H2O	2
OH	2
CH2O	2

Reaction steps	Indices
2 O2 → O + O3	0
CO + O2 → CO2 + O	0
O2 → 2 O	0
H2 + O2 → H + H02	0
2 CO + H2 → 2 HCO	0
CO + H2 → H + HCO	0
H2 → 2 H	0
H02 + O3 → 2 O2 + OH	1
H2 + O3 → H02 + OH	1
H + O3 → O2 + OH	1
O3 → O + O2	1
O + O2 → O3	1
H02 + O2 → O3 + OH	1
H + O2 → O + OH	1
O + O3 → 2 O2	1
H02 + O → O2 + OH	1
HCO + O → CO + OH	1
H2 + O → H + OH	1
H + O → OH	1
CO2 + O → CO + O2	1
2 O → O2	1
HCO + H02 → CH2O + O2	1
H + H02 → 2 OH	1
H + H02 → H2 + O2	1
H + H02 → H2O + O	1
CO + H02 → CO2 + OH	1
HCO + O2 → CO + H02	1
CO + H02 → HCO + O2	1
2 H02 → H2O2 + O2	1
H + O2 → H02	1
H02 → H + O2	1
H2 + H02 → H + H2O2	1
2 HCO → 2 CO + H2	1
H + HCO → CO + H2	1
CO2 + H → CO + OH	1
HCO + O → CO2 + H	1
CO2 + H → HCO + O	1
HCO → CO + H	1
CO + H → HCO	1
H2 + HCO → CH2O + H	1
2 H → H2	1
CO + O → CO2	1
CO2 → CO + O	1
2 HCO → CH2O + CO	1
H + HCO → CH2O	1
2 O2 + OH → H02 + O3	2
H02 + OH → H2 + O3	2
O2 + OH → H + O3	2
O3 + OH → H02 + O2	2
H02 + OH → H2O + O2	2
H2O + O2 → H02 + OH	2
O + OH → H + O2	2
O2 + OH → H02 + O	2
CO + OH → HCO + O	2
H02 + OH → H2O2 + O	2
H2O2 + O → H02 + OH	2
2 OH → H2O + O	2
H2O + O → 2 OH	2
H + OH → H2 + O	2
OH → H + O	2
HCO + OH → CH2O + O	2
CH2O + O → HCO + OH	2
CH2O + O2 → HCO + H02	2
H2O2 + OH → H2O + H02	2



Sun2007

		Reaction steps	Indices
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$2 \text{CO} + \text{H}_2 \rightarrow 2 \text{HCO}$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$\text{HCO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{H} + \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2 \text{HCO} \rightarrow 2 \text{CO} + \text{H}_2$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$2 \text{HCO} \rightarrow \text{CH}_2\text{O} + \text{CO}$	1
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	2
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{OH}$	2
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	2
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	2
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	2
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	2
		$\text{OH} \rightarrow \text{H} + \text{O}$	2
		$\text{CO}_2 + \text{H} + \text{OH} \rightarrow \text{HCO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	2
		$\text{H}_2\text{O}_2 \rightarrow 2 \text{OH}$	2
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	2
		$\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$	2
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	2
		$\text{CO} + \text{H}_2\text{O} \rightarrow \text{HCO} + \text{OH}$	2
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	2
		$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	2

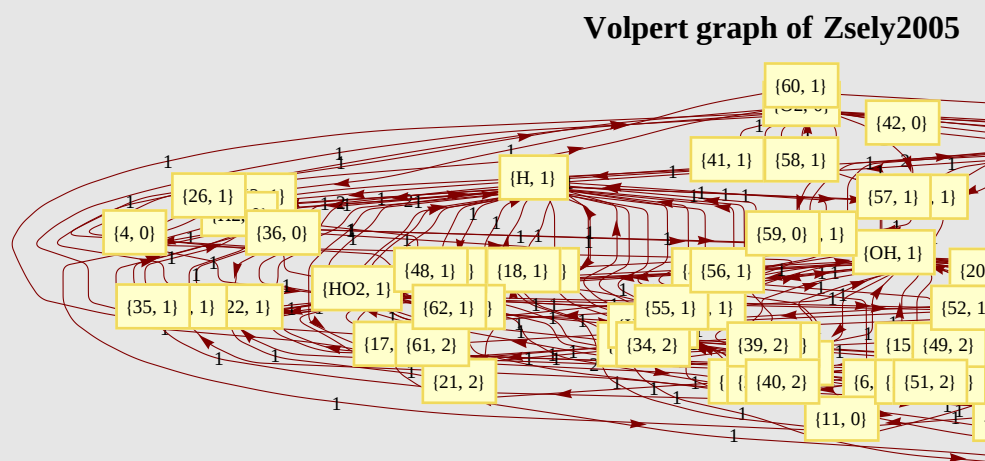


Zsely2005

		Reaction steps	Indices
		$\text{H}_2 + \text{O}_2 \rightarrow 2 \text{OH}$	0
		$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$	0
		$\text{O}_2 \rightarrow 2 \text{O}$	0
		$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2$	0
		$\text{CO} + \text{H}_2 \rightarrow \text{H} + \text{HCO}$	0
		$\text{H}_2 \rightarrow 2 \text{H}$	0
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$	1
		$\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{O}$	1
		$\text{HO}_2 + \text{O} \rightarrow \text{O}_2 + \text{OH}$	1
		$\text{CO} + \text{OH} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{O}$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2 + \text{O}$	1
		$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$	1
		$\text{OH} \rightarrow \text{H} + \text{O}$	1
		$\text{H} + \text{O} \rightarrow \text{OH}$	1
		$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$	1
		$2 \text{O} \rightarrow \text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H} + \text{HO}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow 2 \text{OH}$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	1
		$\text{H} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}$	1
		$\text{CO}_2 + \text{OH} \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1
		$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	1
		$\text{CO} + \text{HO}_2 \rightarrow \text{HCO} + \text{O}_2$	1
		$2 \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1
		$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	1
		$\text{HO}_2 \rightarrow \text{H} + \text{O}_2$	1
		$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$	1
		$2 \text{OH} \rightarrow \text{H}_2\text{O}_2$	1
		$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$	1
		$\text{HCO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	1
		$\text{H} + \text{OH} \rightarrow \text{H}_2\text{O}$	1
		$\text{H} + \text{HCO} \rightarrow \text{CO} + \text{H}_2$	1
		$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	1
		$\text{HCO} + \text{O} \rightarrow \text{CO}_2 + \text{H}$	1
		$\text{CO}_2 + \text{H} \rightarrow \text{HCO} + \text{O}$	1
		$\text{HCO} \rightarrow \text{CO} + \text{H}$	1
		$\text{CO} + \text{H} \rightarrow \text{HCO}$	1
		$2 \text{H} \rightarrow \text{H}_2$	1
		$\text{CO} + \text{O} \rightarrow \text{CO}_2$	1
		$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1
		$\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow 2 \text{OH}$	2
		$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	2
		$\text{H}_2\text{O} + \text{O} \rightarrow \text{H} + \text{HO}_2$	2
		$\text{H}_2\text{O}_2 + \text{O}_2 \rightarrow 2 \text{HO}_2$	2
		$\text{H}_2\text{O} + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}_2$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$	2
		$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	2

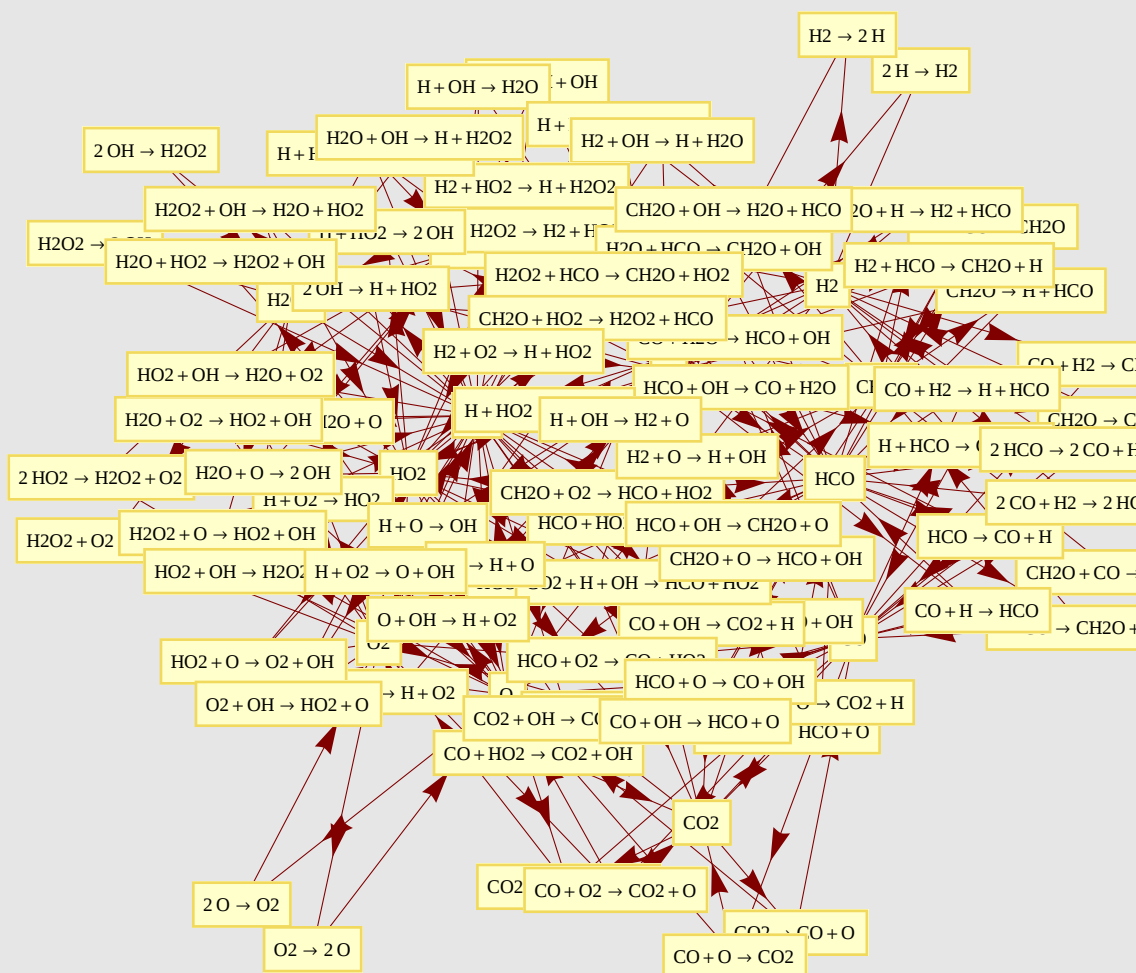
Species	Indices
O2	0
H2	0
CO	0
HO2	1
OH	1
HCO	1
H	1
O	1
CO2	1
H2O2	2
H2O	2

```
ShowVolpertGraph[coevery[[15, 2]], PlotFunction -> "LayeredGraphPlot",
  DirectedEdges -> True, VertexLabeling -> True, ImageSize -> 900,
  PlotLabel -> Style["Volpert graph of "<> coevery[[15, 3]], 15, Bold, Black],
  EdgeLabeling -> True, Numbered -> True, Indexed -> {"H2", "O2", "CO"},
  MultiedgeStyle -> True, PlotRangeClipping -> True]
```



```
ShowVolpertGraph[coevery[[8, 2]], MultiedgeStyle → True,
DirectedEdges → True, VertexLabeling → True,
PlotLabel → Style["Volpert graph of " <> coevery[[2, 3]], 15, Bold, Black],
ImageSize → 600]
```

Volpert graph of CRECK2012



```
ReversibleQ /@ coevery[[reducedindices, 2]]
```

```
{True, False, True, True, True, False, True, True, True, True, True, True}
```

```
db = Sort[DetailedBalanced[#, Total[Length /@ (#1 /. Equal → List)] <
Total[Length /@ (#2 /. Equal → List)] &] & /@
coevery[[Delete[reducedindices, {{2}, {6}}], 2]]
```

```
{ { k2 k8 k9 == k1 k7 k10, k1 k4 k11 == k2 k3 k12, k8 k20 k23 == k7 k19 k24,
k19 k26 k29 == k20 k25 k30, k1 k20 k31 == k2 k19 k32, k8 k36 k45 == k7 k35 k46,
k1 k36 k51 == k2 k35 k52, k20 k35 k71 == k19 k36 k72, k44 k47 k62 == k43 k48 k61,
```

$$\begin{aligned}
& k_{14} k_{15} k_{66} = k_{13} k_{16} k_{65}, k_1 k_4 k_6 k_{13} = k_2 k_3 k_5 k_{14}, k_1 k_4 k_7 k_{17} = k_2 k_3 k_8 k_{18}, \\
& k_1 k_4 k_{20} k_{21} = k_2 k_3 k_{19} k_{22}, k_1 k_7 k_{28} k_{33} = k_2 k_8 k_{27} k_{34}, k_8 k_{27} k_{36} k_{37} = k_7 k_{28} k_{35} k_{38}, \\
& k_1 k_4 k_{36} k_{39} = k_2 k_3 k_{35} k_{40}, k_8 k_{26} k_{27} k_{47} = k_7 k_{25} k_{28} k_{48}, k_5 k_{16} k_{20} k_{61} = k_6 k_{15} k_{19} k_{62}, \\
& k_8 k_{20} k_{27} k_{49} = k_7 k_{19} k_{28} k_{50}, k_2 k_5 k_{16} k_{55} = k_1 k_6 k_{15} k_{56}, k_5 k_7 k_{16} k_{59} = k_6 k_8 k_{15} k_{60}, \\
& k_5 k_{16} k_{36} k_{67} = k_6 k_{15} k_{35} k_{68}, k_8 k_{15} k_{26} k_{27} k_{41} = k_7 k_{16} k_{25} k_{28} k_{42}, \\
& k_5 k_7 k_{16} k_{28} k_{63} = k_6 k_8 k_{15} k_{27} k_{64}, k_5^2 k_7 k_{16}^2 k_{25} k_{28} k_{36} k_{53} = k_6^2 k_8 k_{15}^2 k_{26} k_{27} k_{35} k_{54}, \\
& k_5 k_7 k_{16}^2 k_{25} k_{28} k_{36} k_{57} = k_6 k_8 k_{15}^2 k_{26} k_{27} k_{35} k_{58}, \\
& k_6 k_8 k_{15} k_{26} k_{27} k_{35} k_{69} = k_5 k_7 k_{16} k_{25} k_{28} k_{36} k_{70} \}, \\
& \{ k_4 k_8 k_9 = k_3 k_7 k_{10}, k_5 k_8 k_{13} = k_6 k_7 k_{14}, k_5 k_8^2 k_{15} = k_6 k_7^2 k_{16}, \\
& k_8 k_{18} k_{19} = k_7 k_{17} k_{20}, k_6 k_{18} k_{21} = k_5 k_{17} k_{22}, k_{17} k_{24} k_{27} = k_{18} k_{23} k_{28}, \\
& k_8 k_{30} k_{33} = k_7 k_{29} k_{34}, k_3 k_{12} k_{51} = k_4 k_{11} k_{52}, k_{18} k_{29} k_{67} = k_{17} k_{30} k_{68}, \\
& k_{40} k_{41} k_{66} = k_{39} k_{42} k_{65}, k_{38} k_{41} k_{56} = k_{37} k_{42} k_{55}, k_{10} k_{11} k_{60} = k_9 k_{12} k_{59}, \\
& k_6 k_{25} k_{30} k_{31} = k_5 k_{26} k_{29} k_{32}, k_6 k_{24} k_{25} k_{41} = k_5 k_{23} k_{26} k_{42}, \\
& k_3 k_{12} k_{18} k_{55} = k_4 k_{11} k_{17} k_{56}, k_{24} k_{25} k_{29} k_{65} = k_{23} k_{26} k_{30} k_{66}, \\
& k_6 k_{18} k_{25} k_{43} = k_5 k_{17} k_{26} k_{44}, k_3 k_5 k_{12} k_{53} = k_4 k_6 k_{11} k_{54}, \\
& k_3 k_{12} k_{30} k_{61} = k_4 k_{11} k_{29} k_{62}, k_6 k_{11} k_{24} k_{25} k_{35} = k_5 k_{12} k_{23} k_{26} k_{36}, \\
& k_3 k_5 k_{12} k_{26} k_{57} = k_4 k_6 k_{11} k_{25} k_{58}, k_6 k_7 k_{11} k_{24} k_{25} k_{45} = k_5 k_8 k_{12} k_{23} k_{26} k_{46}, \\
& k_3^2 k_5 k_{12}^2 k_{23} k_{26} k_{30} k_{47} = k_4^2 k_6 k_{11}^2 k_{24} k_{25} k_{29} k_{48}, \\
& k_3 k_5 k_{12}^2 k_{23} k_{26} k_{30} k_{49} = k_4 k_6 k_{11}^2 k_{24} k_{25} k_{29} k_{50}, \\
& k_4 k_6 k_{11} k_{24} k_{25} k_{29} k_{63} = k_3 k_5 k_{12} k_{23} k_{26} k_{30} k_{64} \}, \\
& \{ k_2 k_6 k_7 = k_1 k_5 k_8, k_3 k_6 k_{11} = k_4 k_5 k_{12}, k_6 k_{14} k_{15} = k_5 k_{13} k_{16}, k_4 k_{14} k_{17} = k_3 k_{13} k_{18}, \\
& k_{13} k_{20} k_{23} = k_{14} k_{19} k_{24}, k_6 k_{26} k_{29} = k_5 k_{25} k_{30}, k_4 k_{26} k_{35} = k_3 k_{25} k_{36}, \\
& k_1 k_{10} k_{45} = k_2 k_9 k_{46}, k_{14} k_{25} k_{59} = k_{13} k_{26} k_{60}, k_{34} k_{37} k_{50} = k_{33} k_{38} k_{49}, \\
& k_8 k_9 k_{54} = k_7 k_{10} k_{53}, k_4 k_{21} k_{26} k_{27} = k_3 k_{22} k_{25} k_{28}, k_4 k_{20} k_{21} k_{37} = k_3 k_{19} k_{22} k_{38}, \\
& k_1 k_{10} k_{14} k_{49} = k_2 k_9 k_{13} k_{50}, k_4 k_{14} k_{21} k_{39} = k_3 k_{13} k_{22} k_{40}, k_1 k_3 k_{10} k_{47} = k_2 k_4 k_9 k_{48}, \\
& k_1 k_{10} k_{26} k_{55} = k_2 k_9 k_{25} k_{56}, k_4 k_9 k_{20} k_{21} k_{31} = k_3 k_{10} k_{19} k_{22} k_{32}, \\
& k_1 k_3 k_{10} k_{22} k_{51} = k_2 k_4 k_9 k_{21} k_{52}, k_1^2 k_3 k_{10}^2 k_{19} k_{22} k_{26} k_{41} = k_2^2 k_4 k_9^2 k_{20} k_{21} k_{25} k_{42}, \\
& k_1 k_3 k_{10}^2 k_{19} k_{22} k_{26} k_{43} = k_2 k_4 k_9^2 k_{20} k_{21} k_{25} k_{44}, \\
& k_2 k_4 k_9 k_{20} k_{21} k_{25} k_{57} = k_1 k_3 k_{10} k_{19} k_{22} k_{26} k_{58} \}, \\
& \{ k_4 k_8 k_9 = k_3 k_7 k_{10}, k_8 k_{20} k_{23} = k_7 k_{19} k_{24}, k_{19} k_{26} k_{29} = k_{20} k_{25} k_{30}, \\
& k_3 k_{20} k_{31} = k_4 k_{19} k_{32}, k_8 k_{36} k_{45} = k_7 k_{35} k_{46}, k_3 k_{36} k_{51} = k_4 k_{35} k_{52}, \\
& k_5 k_{16} k_{59} = k_6 k_{15} k_{60}, k_{20} k_{35} k_{73} = k_{19} k_{36} k_{74}, k_{44} k_{47} k_{64} = k_{43} k_{48} k_{63}, \\
& k_{14} k_{15} k_{68} = k_{13} k_{16} k_{67}, k_2 k_3 k_{18} = k_1 k_4 k_{17}, k_1 k_4 k_8 k_{11} = k_2 k_3 k_7 k_{12}, \\
& k_3 k_7 k_{28} k_{33} = k_4 k_8 k_{27} k_{34}, k_8 k_{27} k_{36} k_{37} = k_7 k_{28} k_{35} k_{38}, k_8 k_{26} k_{27} k_{47} = k_7 k_{25} k_{28} k_{48}, \\
& k_5 k_{16} k_{20} k_{63} = k_6 k_{15} k_{19} k_{64}, k_8 k_{20} k_{27} k_{49} = k_7 k_{19} k_{28} k_{50}, \\
& k_4 k_5 k_{16} k_{55} = k_3 k_6 k_{15} k_{56}, k_5 k_7 k_{16} k_{61} = k_6 k_8 k_{15} k_{62}, k_5 k_{16} k_{36} k_{69} = k_6 k_{15} k_{35} k_{70}, \\
& k_1 k_4 k_6 k_8 k_{13} = k_2 k_3 k_5 k_7 k_{14}, k_1 k_4 k_8 k_{20} k_{21} = k_2 k_3 k_7 k_{19} k_{22}, \\
& k_1 k_4 k_8 k_{36} k_{39} = k_2 k_3 k_7 k_{35} k_{40}, k_8 k_{15} k_{26} k_{27} k_{41} = k_7 k_{16} k_{25} k_{28} k_{42}, \\
& k_5 k_7 k_{16} k_{28} k_{65} = k_6 k_8 k_{15} k_{27} k_{66}, k_5^2 k_7 k_{16}^2 k_{25} k_{28} k_{36} k_{53} = k_6^2 k_8 k_{15}^2 k_{26} k_{27} k_{35} k_{54}, \\
& k_5 k_7 k_{16}^2 k_{25} k_{28} k_{36} k_{57} = k_6 k_8 k_{15}^2 k_{26} k_{27} k_{35} k_{58}, \\
& k_6 k_8 k_{15} k_{26} k_{27} k_{35} k_{71} = k_5 k_7 k_{16} k_{25} k_{28} k_{36} k_{72} \}, \\
& \{ k_3 k_6 k_{13} = k_4 k_5 k_{14}, k_1 k_6 k_{21} = k_2 k_5 k_{22}, k_{23} k_{30} k_{33} = k_{24} k_{29} k_{34}, \\
& k_3 k_{24} k_{35} = k_4 k_{23} k_{36}, k_3 k_{40} k_{53} = k_4 k_{39} k_{54}, k_7 k_{18} k_{63} = k_8 k_{17} k_{64}, \\
& k_{24} k_{39} k_{77} = k_{23} k_{40} k_{78}, k_{16} k_{17} k_{72} = k_{15} k_{18} k_{71}, k_2 k_3 k_{20} = k_1 k_4 k_{19}, \\
& k_2 k_3^2 k_6 k_9 = k_1 k_4^2 k_5 k_{10}, k_2 k_3 k_6 k_{11} = k_1 k_4 k_5 k_{12}, k_3 k_6 k_8 k_{15} = k_4 k_5 k_7 k_{16}, \\
& k_3 k_6 k_{24} k_{25} = k_4 k_5 k_{23} k_{26}, k_3 k_6 k_{40} k_{43} = k_4 k_5 k_{39} k_{44}, \\
& k_4 k_7 k_{18} k_{59} = k_3 k_8 k_{17} k_{60}, k_7 k_{18} k_{24} k_{67} = k_8 k_{17} k_{23} k_{68}, \\
& k_7 k_{18} k_{40} k_{73} = k_8 k_{17} k_{39} k_{74}, k_2 k_3^2 k_6 k_{24} k_{27} = k_1 k_4^2 k_5 k_{23} k_{28}, \\
& k_1 k_4 k_5 k_{32} k_{37} = k_2 k_3 k_6 k_{31} k_{38}, k_2 k_3^2 k_6 k_{40} k_{47} = k_1 k_4^2 k_5 k_{39} k_{48}, \\
& k_2 k_3^2 k_6 k_{31} k_{40} k_{41} = k_1 k_4^2 k_5 k_{32} k_{39} k_{42}, k_2 k_3^2 k_6 k_{30} k_{31} k_{49} = k_1 k_4^2 k_5 k_{29} k_{32} k_{50}, \\
& k_2 k_3^2 k_6 k_{24} k_{31} k_{51} = k_1 k_4^2 k_5 k_{23} k_{32} k_{52}, k_2 k_3 k_{17} k_{30} k_{31} k_{55} = k_1 k_4 k_{18} k_{29} k_{32} k_{56},
\end{aligned}$$

$$\begin{aligned}
& k_1 k_4^2 k_5 k_7 k_{18} k_{65} = k_2 k_3^2 k_6 k_8 k_{17} k_{66}, k_2 k_3^2 k_6 k_{17} k_{30} k_{31} k_{45} = k_1 k_4^2 k_5 k_{18} k_{29} k_{32} k_{46}, \\
& k_1 k_4^2 k_5 k_7 k_{18} k_{32} k_{69} = k_2 k_3^2 k_6 k_8 k_{17} k_{31} k_{70}, \\
& k_1 k_4^2 k_5 k_7^2 k_{18}^2 k_{29} k_{32} k_{40} k_{57} = k_2 k_3^2 k_6 k_8^2 k_{17}^2 k_{30} k_{31} k_{39} k_{58}, \\
& k_1 k_4^2 k_5 k_7 k_{18}^2 k_{29} k_{32} k_{40} k_{61} = k_2 k_3^2 k_6 k_8 k_{17}^2 k_{30} k_{31} k_{39} k_{62}, \\
& k_2 k_3^2 k_6 k_8 k_{17} k_{30} k_{31} k_{39} k_{75} = k_1 k_4^2 k_5 k_7 k_{18} k_{29} k_{32} k_{40} k_{76} \}, \\
& \{ k_3 k_6 k_{13} = k_4 k_5 k_{14}, k_{16} k_{24} k_{27} = k_{15} k_{23} k_{28}, k_{23} k_{32} k_{37} = k_{24} k_{31} k_{38}, \\
& k_3 k_{24} k_{39} = k_4 k_{23} k_{40}, k_{16} k_{44} k_{51} = k_{15} k_{43} k_{52}, k_3 k_{44} k_{61} = k_4 k_{43} k_{62}, \\
& k_7 k_{20} k_{73} = k_8 k_{19} k_{74}, k_{24} k_{43} k_{87} = k_{23} k_{44} k_{88}, k_{54} k_{57} k_{78} = k_{53} k_{58} k_{77}, \\
& k_{18} k_{19} k_{82} = k_{17} k_{20} k_{81}, k_{16} k_{19} k_{66} = k_{15} k_{20} k_{65}, k_2 k_3 k_{22} = k_1 k_4 k_{21}, \\
& k_2 k_3^2 k_6 k_9 = k_1 k_4^2 k_5 k_{10}, k_2 k_3 k_6 k_{11} = k_1 k_4 k_5 k_{12}, k_3 k_6 k_8 k_{17} = k_4 k_5 k_7 k_{18}, \\
& k_3 k_6 k_{24} k_{25} = k_4 k_5 k_{23} k_{26}, k_{16} k_{19} k_{32} k_{33} = k_{15} k_{20} k_{31} k_{34}, \\
& k_3 k_6 k_{44} k_{47} = k_4 k_5 k_{43} k_{48}, k_7 k_{20} k_{24} k_{77} = k_8 k_{19} k_{23} k_{78}, k_4 k_7 k_{20} k_{69} = k_3 k_8 k_{19} k_{70}, \\
& k_7 k_{20} k_{44} k_{83} = k_8 k_{19} k_{43} k_{84}, k_2 k_3^2 k_6 k_{24} k_{29} = k_1 k_4^2 k_5 k_{23} k_{30}, \\
& k_1 k_4 k_5 k_{36} k_{41} = k_2 k_3 k_6 k_{35} k_{42}, k_2 k_3^2 k_6 k_{44} k_{55} = k_1 k_4^2 k_5 k_{43} k_{56}, \\
& k_2 k_3^2 k_6 k_{35} k_{44} k_{45} = k_1 k_4^2 k_5 k_{36} k_{43} k_{46}, k_2 k_3^2 k_6 k_{32} k_{35} k_{57} = k_1 k_4^2 k_5 k_{31} k_{36} k_{58}, \\
& k_2 k_3^2 k_6 k_{24} k_{35} k_{59} = k_1 k_4^2 k_5 k_{23} k_{36} k_{60}, k_2 k_3 k_{19} k_{32} k_{35} k_{63} = k_1 k_4 k_{20} k_{31} k_{36} k_{64}, \\
& k_1 k_4^2 k_5 k_7 k_{20} k_{75} = k_2 k_3^2 k_6 k_8 k_{19} k_{76}, k_2 k_3^2 k_6 k_{19} k_{32} k_{35} k_{49} = k_1 k_4^2 k_5 k_{20} k_{31} k_{36} k_{50}, \\
& k_1 k_4^2 k_5 k_7 k_{20} k_{36} k_{79} = k_2 k_3^2 k_6 k_8 k_{19} k_{35} k_{80}, \\
& k_1 k_4^2 k_5 k_7^2 k_{20}^2 k_{31} k_{36} k_{44} k_{67} = k_2 k_3^2 k_6 k_8^2 k_{19}^2 k_{32} k_{35} k_{43} k_{68}, \\
& k_1 k_4^2 k_5 k_7 k_{20}^2 k_{31} k_{36} k_{44} k_{71} = k_2 k_3^2 k_6 k_8 k_{19}^2 k_{32} k_{35} k_{43} k_{72}, \\
& k_2 k_3^2 k_6 k_8 k_{19} k_{32} k_{35} k_{43} k_{85} = k_1 k_4^2 k_5 k_7 k_{20} k_{31} k_{36} k_{44} k_{86} \}, \\
& \{ k_2 k_6 k_7 = k_1 k_5 k_8, k_4 k_{10} k_{11} = k_3 k_9 k_{12}, k_5 k_{10} k_{15} = k_6 k_9 k_{16}, \\
& k_{10} k_{18} k_{19} = k_9 k_{17} k_{20}, k_6 k_{18} k_{21} = k_5 k_{17} k_{22}, k_{17} k_{24} k_{27} = k_{18} k_{23} k_{28}, \\
& k_1 k_{18} k_{29} = k_2 k_{17} k_{30}, k_{10} k_{34} k_{39} = k_9 k_{33} k_{40}, k_6 k_{34} k_{45} = k_5 k_{33} k_{46}, \\
& k_1 k_{34} k_{51} = k_2 k_{33} k_{52}, k_3 k_{14} k_{59} = k_4 k_{13} k_{60}, k_{18} k_{33} k_{73} = k_{17} k_{34} k_{74}, \\
& k_{44} k_{47} k_{64} = k_{43} k_{48} k_{63}, k_{34} k_{35} k_{72} = k_{33} k_{36} k_{71}, k_{12} k_{13} k_{68} = k_{11} k_{14} k_{67}, \\
& k_1 k_5 k_{26} k_{31} = k_2 k_6 k_{25} k_{32}, k_6 k_{25} k_{34} k_{37} = k_5 k_{26} k_{33} k_{38}, \\
& k_6 k_{24} k_{25} k_{47} = k_5 k_{23} k_{26} k_{48}, k_3 k_{14} k_{18} k_{63} = k_4 k_{13} k_{17} k_{64}, \\
& k_6 k_{18} k_{25} k_{49} = k_5 k_{17} k_{26} k_{50}, k_2 k_3 k_{14} k_{55} = k_1 k_4 k_{13} k_{56}, k_3 k_5 k_{14} k_{61} = k_4 k_6 k_{13} k_{62}, \\
& k_3 k_{14} k_{34} k_{69} = k_4 k_{13} k_{33} k_{70}, k_6 k_{13} k_{24} k_{25} k_{41} = k_5 k_{14} k_{23} k_{26} k_{42}, \\
& k_3 k_5 k_{14} k_{26} k_{65} = k_4 k_6 k_{13} k_{25} k_{66}, k_4 k_6 k_{13} k_{24} k_{25} k_{35} = k_3 k_5 k_{14} k_{23} k_{26} k_{36}, \\
& k_3^2 k_5 k_{14}^2 k_{23} k_{26} k_{34} k_{53} = k_4^2 k_6 k_{13}^2 k_{24} k_{25} k_{33} k_{54}, \\
& k_3 k_5 k_{14}^2 k_{23} k_{26} k_{34} k_{57} = k_4 k_6 k_{13}^2 k_{24} k_{25} k_{33} k_{58} \}, \\
& \{ k_1 k_4 k_9 = k_2 k_3 k_{10}, k_4 k_{12} k_{13} = k_3 k_{11} k_{14}, k_2 k_{12} k_{15} = k_1 k_{11} k_{16}, \\
& k_{11} k_{18} k_{21} = k_{12} k_{17} k_{22}, k_4 k_{24} k_{29} = k_3 k_{23} k_{30}, k_2 k_{24} k_{35} = k_1 k_{23} k_{36}, \\
& k_{12} k_{23} k_{59} = k_{11} k_{24} k_{60}, k_{34} k_{37} k_{50} = k_{33} k_{38} k_{49}, k_{24} k_{25} k_{58} = k_{23} k_{26} k_{57}, \\
& k_6 k_7 k_{54} = k_5 k_8 k_{53}, k_2 k_{19} k_{24} k_{27} = k_1 k_{20} k_{23} k_{28}, k_2 k_{18} k_{19} k_{37} = k_1 k_{17} k_{20} k_{38}, \\
& k_2 k_{12} k_{19} k_{39} = k_1 k_{11} k_{20} k_{40}, k_4 k_5 k_8 k_{45} = k_3 k_6 k_7 k_{46}, \\
& k_2 k_7 k_{18} k_{19} k_{31} = k_1 k_8 k_{17} k_{20} k_{32}, k_4 k_5 k_8 k_{12} k_{49} = k_3 k_6 k_7 k_{11} k_{50}, \\
& k_1 k_4 k_5 k_8 k_{47} = k_2 k_3 k_6 k_7 k_{48}, k_4 k_5 k_8 k_{24} k_{55} = k_3 k_6 k_7 k_{23} k_{56}, \\
& k_1 k_4 k_5 k_8 k_{20} k_{51} = k_2 k_3 k_6 k_7 k_{19} k_{52}, k_2 k_3 k_6 k_7 k_{18} k_{19} k_{25} = k_1 k_4 k_5 k_8 k_{17} k_{20} k_{26}, \\
& k_1 k_4^2 k_5^2 k_8^2 k_{17} k_{20} k_{24} k_{41} = k_2 k_3^2 k_6^2 k_7^2 k_{18} k_{19} k_{23} k_{42}, \\
& k_1 k_4 k_5 k_8^2 k_{17} k_{20} k_{24} k_{43} = k_2 k_3 k_6 k_7^2 k_{18} k_{19} k_{23} k_{44} \}, \\
& \{ k_2 k_8 k_9 = k_1 k_7 k_{10}, k_1 k_4 k_{11} = k_2 k_3 k_{12}, k_8 k_{22} k_{25} = k_7 k_{21} k_{26}, \\
& k_{21} k_{28} k_{31} = k_{22} k_{27} k_{32}, k_1 k_{22} k_{33} = k_2 k_{21} k_{34}, k_8 k_{38} k_{47} = k_7 k_{37} k_{48}, \\
& k_1 k_{38} k_{53} = k_2 k_{37} k_{54}, k_5 k_{16} k_{61} = k_6 k_{15} k_{62}, k_{22} k_{37} k_{77} = k_{21} k_{38} k_{78}, \\
& k_{46} k_{49} k_{66} = k_{45} k_{50} k_{65}, k_{14} k_{15} k_{70} = k_{13} k_{16} k_{69}, k_1 k_4 k_6 k_{13} = k_2 k_3 k_5 k_{14}, \\
& k_1 k_4 k_7 k_{17} = k_2 k_3 k_8 k_{18}, k_1^2 k_4^2 k_7 k_{19} = k_2^2 k_3^2 k_8 k_{20}, k_1 k_4 k_{22} k_{23} = k_2 k_3 k_{21} k_{24}, \\
& k_1 k_7 k_{30} k_{35} = k_2 k_8 k_{29} k_{36}, k_8 k_{29} k_{38} k_{39} = k_7 k_{30} k_{37} k_{40}, \\
& k_1 k_4 k_{38} k_{41} = k_2 k_3 k_{37} k_{42}, k_8 k_{28} k_{29} k_{49} = k_7 k_{27} k_{30} k_{50}, \\
& k_5 k_{16} k_{22} k_{65} = k_6 k_{15} k_{21} k_{66}, k_8 k_{22} k_{29} k_{51} = k_7 k_{21} k_{30} k_{52},
\end{aligned}$$

$$\begin{aligned}
& k_2 k_5 k_{16} k_{57} = k_1 k_6 k_{15} k_{58}, k_5 k_7 k_{16} k_{63} = k_6 k_8 k_{15} k_{64}, k_5 k_{16} k_{38} k_{71} = k_6 k_{15} k_{37} k_{72}, \\
& k_8 k_{15} k_{28} k_{29} k_{43} = k_7 k_{16} k_{27} k_{30} k_{44}, k_5 k_7 k_{16} k_{30} k_{67} = k_6 k_8 k_{15} k_{29} k_{68}, \\
& k_5 k_{16} k_{38} k_{74} k_{79} = k_6 k_{15} k_{37} k_{73} k_{80}, k_5^2 k_7 k_{16}^2 k_{27} k_{30} k_{38} k_{55} = k_6^2 k_8 k_{15}^2 k_{28} k_{29} k_{37} k_{56}, \\
& k_5 k_7 k_{16}^2 k_{27} k_{30} k_{38} k_{59} = k_6 k_8 k_{15}^2 k_{28} k_{29} k_{37} k_{60}, \\
& k_6 k_8 k_{15} k_{28} k_{29} k_{37} k_{75} = k_5 k_7 k_{16} k_{27} k_{30} k_{38} k_{76}, \\
& k_6 k_{15} k_{28} k_{29} k_{37}^2 k_{73} k_{85} = k_5 k_{16} k_{27} k_{30} k_{38}^2 k_{74} k_{86}, \\
& k_6 k_8 k_{15} k_{28} k_{29} k_{73} k_{87} = k_5 k_7 k_{16} k_{27} k_{30} k_{74} k_{88}, \\
& k_5^2 k_7 k_{16}^2 k_{27} k_{30} k_{38} k_{74} k_{81} = k_6^2 k_8 k_{15}^2 k_{28} k_{29} k_{37} k_{73} k_{82}, \\
& k_6 k_8 k_{15} k_{28} k_{29} k_{37} k_{73} k_{83} = k_5 k_7 k_{16} k_{27} k_{30} k_{38} k_{74} k_{84} \}, \\
& \{ k_4 k_8 k_9 = k_3 k_7 k_{10}, k_5 k_8 k_{13} = k_6 k_7 k_{14}, k_5 k_8^2 k_{15} = k_6 k_7^2 k_{16}, \\
& k_8 k_{18} k_{19} = k_7 k_{17} k_{20}, k_6 k_{18} k_{21} = k_5 k_{17} k_{22}, k_{17} k_{24} k_{27} = k_{18} k_{23} k_{28}, \\
& k_8 k_{30} k_{33} = k_7 k_{29} k_{34}, k_6 k_{30} k_{39} = k_5 k_{29} k_{40}, k_3 k_{12} k_{51} = k_4 k_{11} k_{52}, \\
& k_{18} k_{29} k_{65} = k_{17} k_{30} k_{66}, k_{38} k_{41} k_{56} = k_{37} k_{42} k_{55}, k_{10} k_{11} k_{60} = k_9 k_{12} k_{59}, \\
& k_6 k_{25} k_{30} k_{31} = k_5 k_{26} k_{29} k_{32}, k_6 k_{24} k_{25} k_{41} = k_5 k_{23} k_{26} k_{42}, \\
& k_3 k_{12} k_{18} k_{55} = k_4 k_{11} k_{17} k_{56}, k_6 k_{18} k_{25} k_{43} = k_5 k_{17} k_{26} k_{44}, k_3 k_5 k_{12} k_{53} = k_4 k_6 k_{11} k_{54}, \\
& k_3 k_{12} k_{30} k_{61} = k_4 k_{11} k_{29} k_{62}, k_6 k_{11} k_{24} k_{25} k_{35} = k_5 k_{12} k_{23} k_{26} k_{36}, \\
& k_3 k_5 k_{12} k_{26} k_{57} = k_4 k_6 k_{11} k_{25} k_{58}, k_6 k_7 k_{11} k_{24} k_{25} k_{45} = k_5 k_8 k_{12} k_{23} k_{26} k_{46}, \\
& k_3^2 k_5 k_{12}^2 k_{23} k_{26} k_{30} k_{47} = k_4^2 k_6 k_{11}^2 k_{24} k_{25} k_{29} k_{48}, \\
& k_3 k_5 k_{12}^2 k_{23} k_{26} k_{30} k_{49} = k_4 k_6 k_{11}^2 k_{24} k_{25} k_{29} k_{50}, \\
& k_4 k_6 k_{11} k_{24} k_{25} k_{29} k_{63} = k_3 k_5 k_{12} k_{23} k_{26} k_{30} k_{64} \}, \\
& \{ k_2 k_6 k_7 = k_1 k_5 k_8, k_3 k_6 k_{11} = k_4 k_5 k_{12}, k_6 k_{14} k_{15} = k_5 k_{13} k_{16}, k_4 k_{14} k_{17} = k_3 k_{13} k_{18}, \\
& k_{13} k_{20} k_{23} = k_{14} k_{19} k_{24}, k_6 k_{26} k_{29} = k_5 k_{25} k_{30}, k_1 k_{10} k_{45} = k_2 k_9 k_{46}, \\
& k_{14} k_{25} k_{61} = k_{13} k_{26} k_{62}, k_{36} k_{37} k_{60} = k_{35} k_{38} k_{59}, k_{34} k_{37} k_{50} = k_{33} k_{38} k_{49}, \\
& k_8 k_9 k_{54} = k_7 k_{10} k_{53}, k_4 k_{21} k_{26} k_{27} = k_3 k_{22} k_{25} k_{28}, k_4 k_{20} k_{21} k_{37} = k_3 k_{19} k_{22} k_{38}, \\
& k_1 k_{10} k_{14} k_{49} = k_2 k_9 k_{13} k_{50}, k_{20} k_{21} k_{25} k_{59} = k_{19} k_{22} k_{26} k_{60}, \\
& k_4 k_{14} k_{21} k_{39} = k_3 k_{13} k_{22} k_{40}, k_1 k_3 k_{10} k_{47} = k_2 k_4 k_9 k_{48}, \\
& k_1 k_{10} k_{26} k_{55} = k_2 k_9 k_{25} k_{56}, k_4 k_9 k_{20} k_{21} k_{31} = k_3 k_{10} k_{19} k_{22} k_{32}, \\
& k_1 k_3 k_{10} k_{22} k_{51} = k_2 k_4 k_9 k_{21} k_{52}, k_1^2 k_3 k_{10}^2 k_{19} k_{22} k_{26} k_{41} = k_2^2 k_4 k_9^2 k_{20} k_{21} k_{25} k_{42}, \\
& k_1 k_3 k_{10}^2 k_{19} k_{22} k_{26} k_{43} = k_2 k_4 k_9^2 k_{20} k_{21} k_{25} k_{44}, \\
& k_2 k_4 k_9 k_{20} k_{21} k_{25} k_{57} = k_1 k_3 k_{10} k_{19} k_{22} k_{26} k_{58} \} \}
\end{aligned}$$

```
TableForm[db,
  TableHeadings → {coevery[Delete[reducedindices, {{2}, {6}}], 3]}]
```

```
TableForm[Table[Complement[
  ReactionsData[coevery[i, 2], ExternalSpecies → "HV"] ["fhjgraph"],
  ReactionsData[coevery[j, 2], ExternalSpecies → "HV"] ["fhjgraph"]],
  {i, reducedindices}, {j, reducedindices}],
  TableHeadings → {coevery[reducedindices, 3], coevery[reducedindices, 3]}]
```

```
TableForm[Table[Length@Complement[
  ReactionsData[coevery[[i, 2]], ExternalSpecies → {"HV"}][["fhjgraph"]],
  ReactionsData[coevery[[j, 2]], ExternalSpecies → "HV"][["fhjgraph"]],
  {i, reducedindices}, {j, reducedindices}], TableHeadings →
  {coevery[[reducedindices, 3]], coevery[[reducedindices, 3]]}]
```

	Ahmed2007	CRECK2012	Dagaut2003	Davis2005	gri30
Ahmed2007	0	19	12	14	2
CRECK2012	7	0	6	7	7
Dagaut2003	8	14	0	8	8
Davis2005	2	7	0	0	0
gri30	4	21	14	14	0
Keromnes2013	8	10	4	6	6
Li2007	8	24	14	20	6
Rasmussen2008	16	34	24	28	14
SanDiego2011	4	19	14	14	2
SaxenaWilliams2006	4	7	2	2	2
Starik2009	16	35	24	28	16
Sun2007	6	12	0	6	6
Zsely2005	4	9	0	2	2

Methanol combustion mechanisms

```
SetDirectory[NotebookDirectory[] <> "methanol"];
```

```
ClearAll[mdata];
mdat = Flatten[Import["names_methanol.txt", "Table"]];
mdata = StringReplace[#, ".dat" → ""] & /@ mdat
```

```
{Aranda2013, Klippenstein2011, Li2007, Rasmussen2008, ZabettaHuba2008}
```

```
indices = Range[5];
```

```
TableForm[mdata, TableHeadings → {indices, None}]
```

```
1 | Aranda2013
2 | Klippenstein2011
3 | Li2007
4 | Rasmussen2008
5 | ZabettaHuba2008
```

```
ClearAll[mall];
mall = CHEMKINImport[#]["chemkinreactions"] & /@ mdat; // AbsoluteTiming
```

```
{2.8941656, Null}
```

```
ClearAll[mevery];
mevery = Transpose[{mall, DeleteAutocatalysis /@ mall, mdata}]; //
AbsoluteTiming
```

```
{3.2371851, Null}
```

```
TableForm[ReactionsData[#][{"M", "R", "deficiency"}] & /@ mevery[[indices, 2]],
TableHeadings → {mevery[[indices, 3]], {"M", "R", "deficiency"}}]
```

	M	R	deficiency
Aranda2013	76	1063	$\delta = n-l-s = 661-187-71 = 403$
Klippenstein2011	18	172	$\delta = n-l-s = 122-42-15 = 65$
Li2007	18	170	$\delta = n-l-s = 121-42-15 = 64$
Rasmussen2008	28	320	$\delta = n-l-s = 222-75-24 = 123$
ZabettaHuba2008	58	724	$\delta = n-l-s = 500-163-54 = 283$

```
TableForm[ReactionsData[#][{"species"}] & /@ mevery[[indices, 2]],
TableHeadings → {mevery[[indices, 3]], {"list", " of ", "species\n"}}]
```

	list	of	species
Aranda2013	CH200H	CH2O	OH C2H4 HOCH2CH200 CH2OH
Klippenstein2011	C2H6	CH3	CH2O CO H2 H
Li2007	C2H6	CH3	CH2O CO H2 H
Rasmussen2008	NO2	NO2*	NO O2 CH2O CO
ZabettaHuba2008	C2H2	C2H	H C4H2 C2H3 C2H4

```
TableForm[Table[mevery[[i, 2]] /. x_Equilibrium → Sequence[], {i, 5}],
TableHeadings → {mevery[[indices, 3]], None}]
```

Aranda2013	CH200H → CH2O + OH	C2H4 + HOCH2CH200 → CH2O + CH2OH + CH3CHO
Klippenstein2011		
Li2007		
Rasmussen2008	NO2 → NO2*	2 NO2* → 2 NO + O2
ZabettaHuba2008		

```
mevery[[1, 2]] /. x_Equilibrium → Sequence[]
```

```
{CH200H → CH2O + OH, C2H4 + HOCH2CH200 → CH2O + CH2OH + CH3CHO,
CH2O + HOCH2CH200 → CH2OH + CH200H + HCO,
HO2 + HOCH2CH200 → CH2OH + CH200H + O2, CH2CHOH + O2 → CH2O + HCO + OH}
```

```
mevery[[-2, 2]] /. x_Equilibrium → Sequence[]
```

```
{NO2 → NO2*, 2 NO2* → 2 NO + O2}
```

```
Row[{ShowFHJGraph[#[[2]], DirectedEdges → True,
VertexLabeling → All, PlotLabel → #[[3]], ImageSize → 420], " ",
Column[Join[{"3rd body species deleted"}, #[[2]]]], " ", Column[
Join[{"Orig. Mechanism"}, #[[1]]]]] & /@ mevery[[indices]] // Timing
```

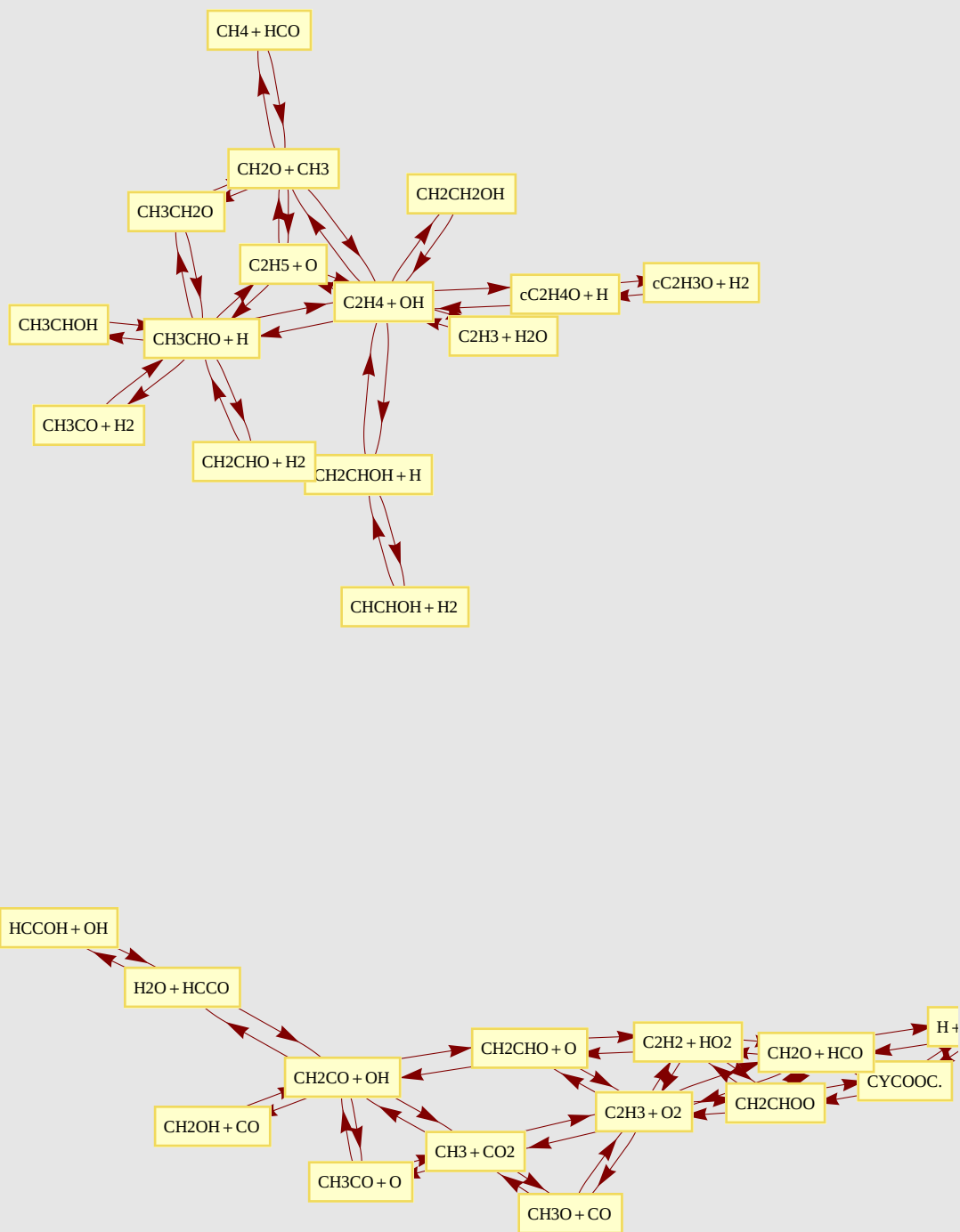
```
maxfhjcomponents = MaxFHJWeaklyConnectedComponents[mevery[[#, 2]] & /@  
  indices; // AbsoluteTiming
```

```
{0.0040002, Null}
```

```
maxfhjedges = Flatten[First /@#] & /@maxfhjcomponents;
```

```
GraphPlot[First[#], VertexLabeling → True, DirectedEdges → True,  
  ImageSize → 700, PlotLabel → "Max weakly connected component of mech " <>  
  ToString[mevery[[Last[#], 3]] <> "\n"] & /@  
  Transpose[{maxfhjedges, indices}]
```

Max weakly connected component of mech Aranda2013



```
TableForm[
  tt = Table[TrueQ[mevery[[i, 2]] == mevery[[j, 2]]] /. {True → Style["TRUE", Bold]},
    {i, 5}, {j, 5}], TableHeadings → {mdata, mdata}]
```

	Aranda2013	Klippenstein2011	Li2007	Rasmussen2008
Aranda2013	TRUE	False	False	False
Klippenstein2011	False	TRUE	False	False
Li2007	False	False	TRUE	False
Rasmussen2008	False	False	False	TRUE
ZabettaHuba2008	False	False	False	False

```
ag = (tt /. {Style["TRUE", Bold] → 1, False → 0}) - IdentityMatrix[5];
```

```
AdjacencyGraph[ag, ImageSize → 550, ImagePadding → 60, VertexLabels →
  Thread[Rule[indices, Style[#, Bold, 12] & /@ mevery[[indices, 3]]]]]
```



```
reducedindices = Sort[First /@ ConnectedComponents[AdjacencyGraph[ag]]]
```

```
{1, 2, 3, 4, 5}
```

```
Column[Riffle[Row /@
  (Join[{Style[mevery[[#, 3]], Bold, 14], "\t"}, VolpertIndexing[mevery[[#, 2]],
    {"CH2O"}, Verbose → True]] & /@ reducedindices), "\n\n"], 2]
```

```
Column[
  Riffle[Row /@ (Join[{Style[mevery[[#, 3]], Bold, 14], "\t"}, VolpertIndexing[
    mevery[[#, 2]], {"CH3OH", "O2", "N2"},
    Verbose → True]] & /@ reducedindices), "\n\n"], 2]
```

```
ShowVolpertGraph[mevery[[3, 2]], PlotFunction → "LayeredGraphPlot",
  DirectedEdges → True, VertexLabeling → True, ImageSize → 1000,
  PlotLabel → Style["Volpert graph of " <> mevery[[3, 3]], 15, Bold, Black],
  EdgeLabeling → True, Numbered → True, Indexed → {"CH3OH", "O2", "N2"},
  MultiedgeStyle → True, PlotRangeClipping → True]
```

```
ReversibleQ /@ mevery[[reducedindices, 2]]
```

```
{False, True, True, False, True}
```

```
db = Sort[DetailedBalanced[#, Total[Length /@ (#1 /. Equal → List)] <
      Total[Length /@ (#2 /. Equal → List)] &] & /@
      mevery[Delete[reducedindices, {{1}, {4}}], 2]; // AbsoluteTiming
```

```
{14.5088299, Null}
```

```
TableForm[db, TableHeadings → {mevery[Delete[reducedindices, {{1}, {4}}], 3}}]
```

Klippenstein2011	$k_6 k_7 k_{11} = k_5 k_8 k_{12}$	$k_8 k_{14} k_{15} = k_7 k_{13} k_{16}$	$k_9^2 k_{14} k_{21} = k_1^2$
Li2007	$k_6 k_7 k_{11} = k_5 k_8 k_{12}$	$k_8 k_{14} k_{15} = k_7 k_{13} k_{16}$	$k_9^2 k_{14} k_{21} = k_1^2$
ZabettaHuba2008	$k_{17} k_{24} k_{27} = k_{18} k_{23} k_{28}$	$k_{18} k_{50} k_{51} = k_{17} k_{49} k_{52}$	$k_{39}^2 k_{44} k_{71} = k$

```
TableForm[Table[Complement[ReactionsData[mevery[i, 2]]["fhjgraph"],
      ReactionsData[mevery[j, 2]]["fhjgraph"]],
      {i, reducedindices}, {j, reducedindices}],
      TableHeadings → {mevery[reducedindices, 3], mevery[reducedindices, 3]}]
```

```
TableForm[Table[Length@Complement[ReactionsData[mevery[i, 2]]["fhjgraph"],
      ReactionsData[mevery[j, 2]]["fhjgraph"]],
      {i, reducedindices}, {j, reducedindices}],
      TableHeadings → {mevery[reducedindices, 3], mevery[reducedindices, 3]}]
```

	Aranda2013	Klippenstein2011	Li2007	Rasmussen2008
Aranda2013	0	897	899	759
Klippenstein2011	6	0	2	8
Li2007	6	0	0	6
Rasmussen2008	16	156	156	0
ZabettaHuba2008	398	570	570	524