Supplementary information for

Mechanisms and Kinetic Studies of OH-initiated Atmospheric Oxidation of Methoxyphenols in the Presence of O_2 and NO_x

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Nineteen pages

Contains six tables and ten figures

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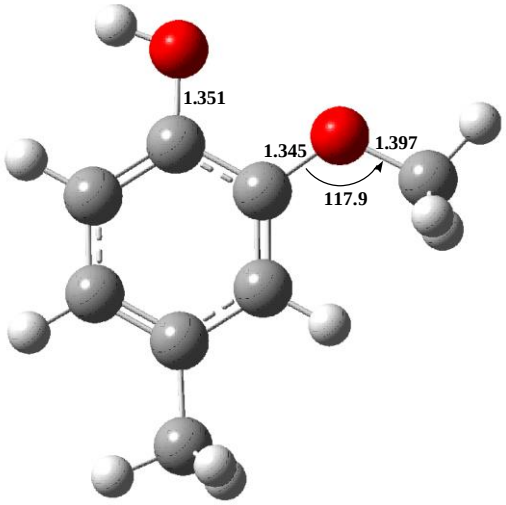
Figure S1. MPWB1K/6-31+G(d,p) optimized geometric conformers of creosol. Distances are in angstrom, and angles are in degree.



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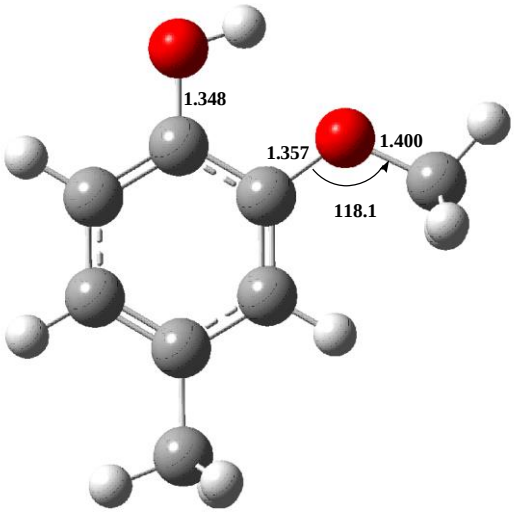

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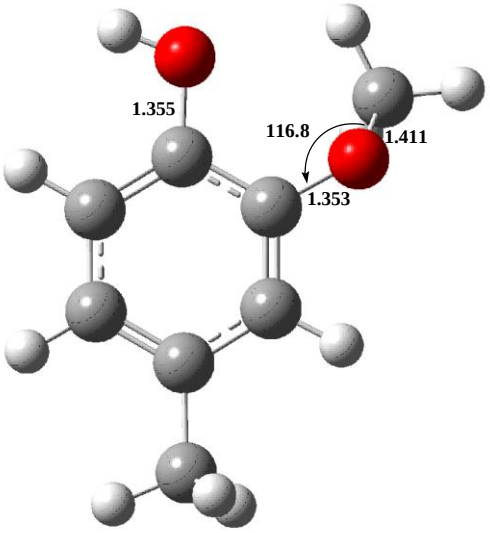

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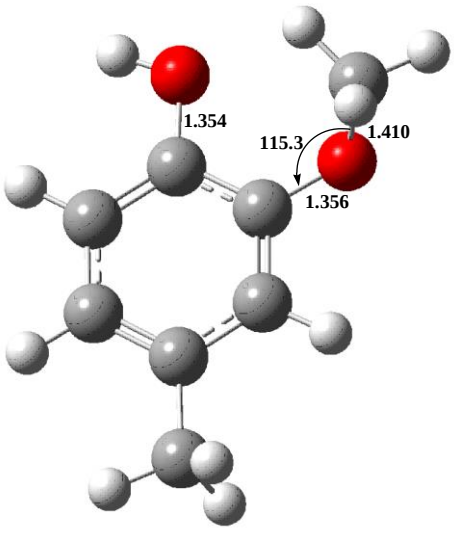

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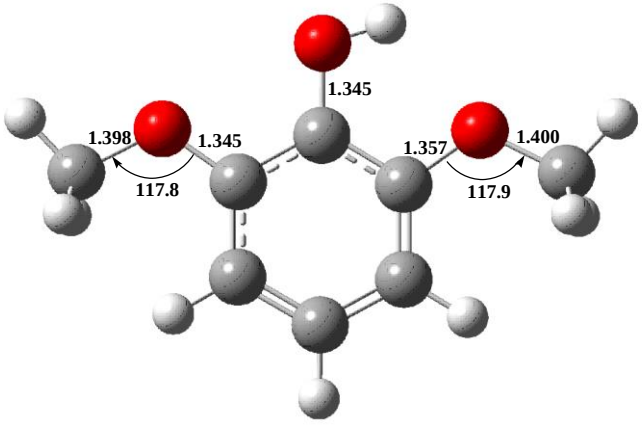
Structure Ⅱ	0.169656	-461.2345621	0

Structure Ⅲ	0.169121	-461.2244296	6.02
Structure Ⅴ	0.169342	-461.2248788	5.88

Figure S2. MPWB1K/6-31+G(d,p) optimized geometric conformers of syringol. Distances are in angstrom, and angles are in degree.



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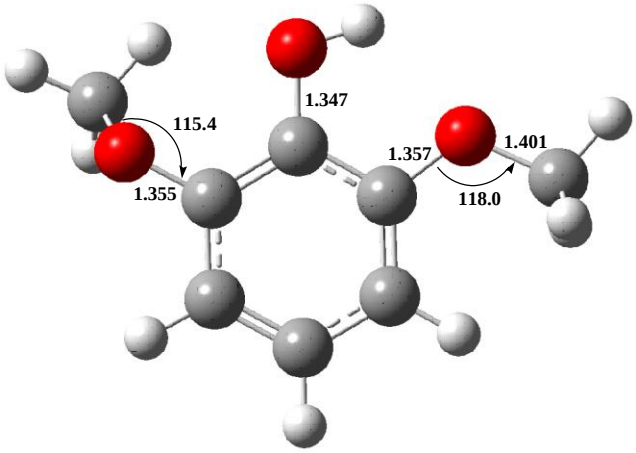

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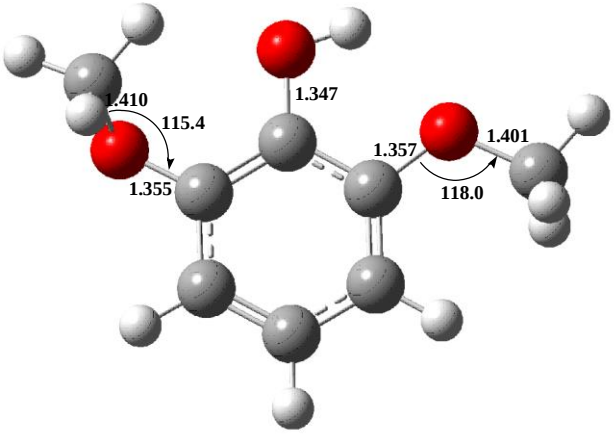

Structure Ⅲ

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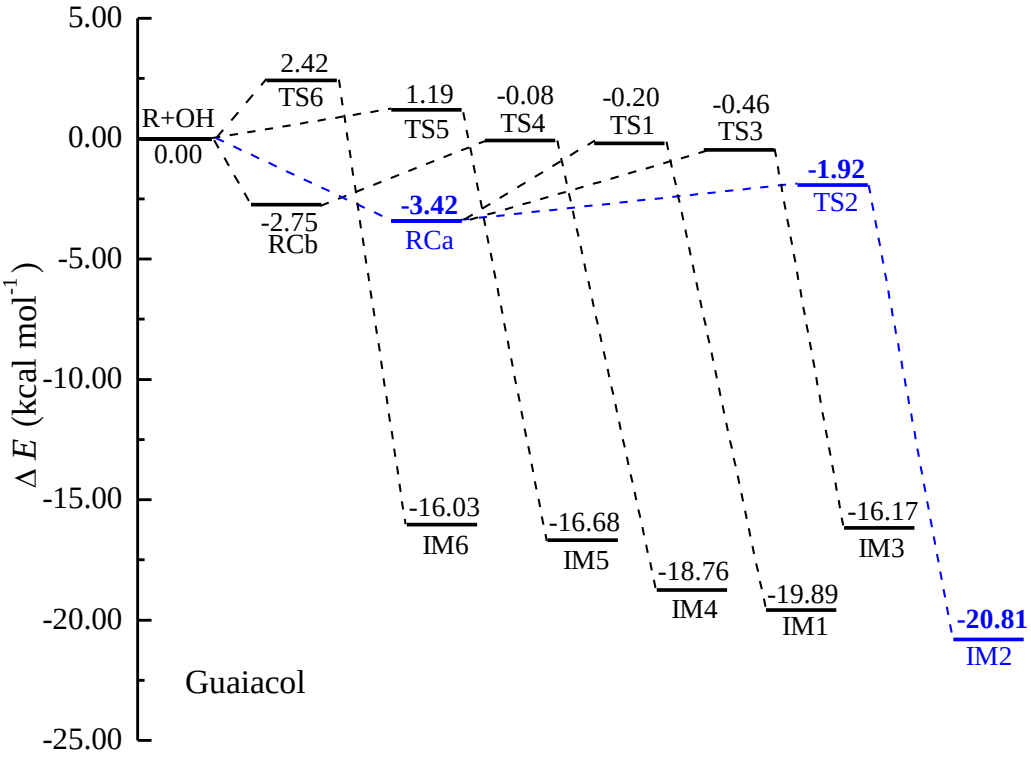
Structure Ⅱ	0.175425	-536.4344257	1.05
Structure Ⅲ	0.175422	-536.4344242	1.05

Figure S3. Profile of the potential energy surface for the reaction of guaiacol with OH radicals at the MPWB1K/6-311+G(3df,2p) level.



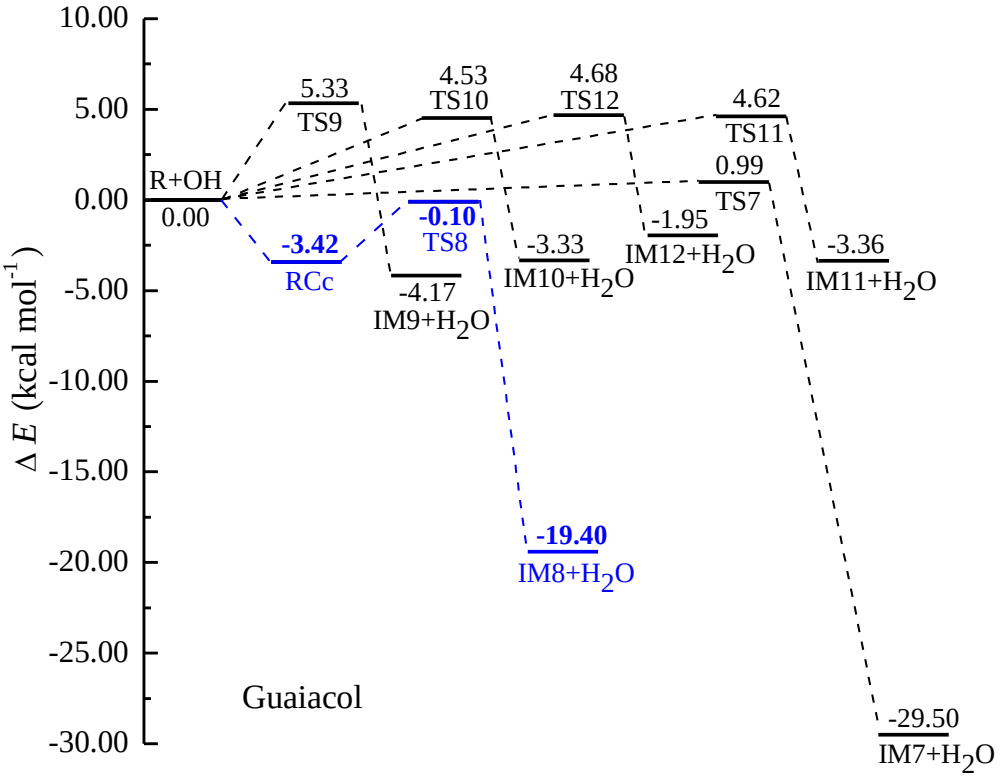


Figure S4. OH radical-initiated reaction scheme of creosol embedded with the potential barriers $\triangle E$ (kcal mol^{-1}) and reaction heats $\triangle H$ (kcal mol^{-1})

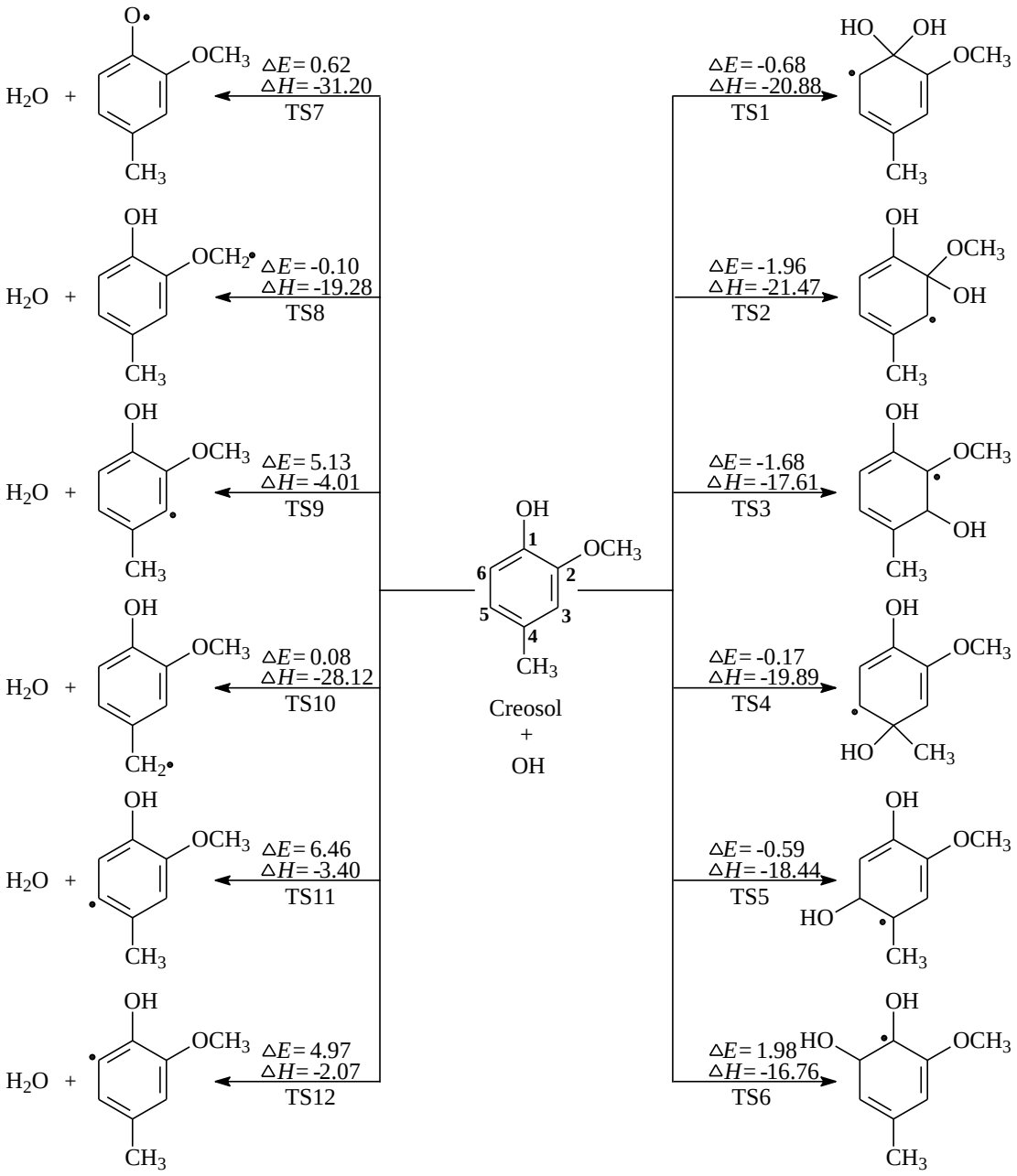


Figure S5. OH radical-initiated reaction scheme of syringol embedded with the potential barriers $\triangle E$ (kcal mol^{-1}) and reaction heats $\triangle H$ (kcal mol^{-1}).

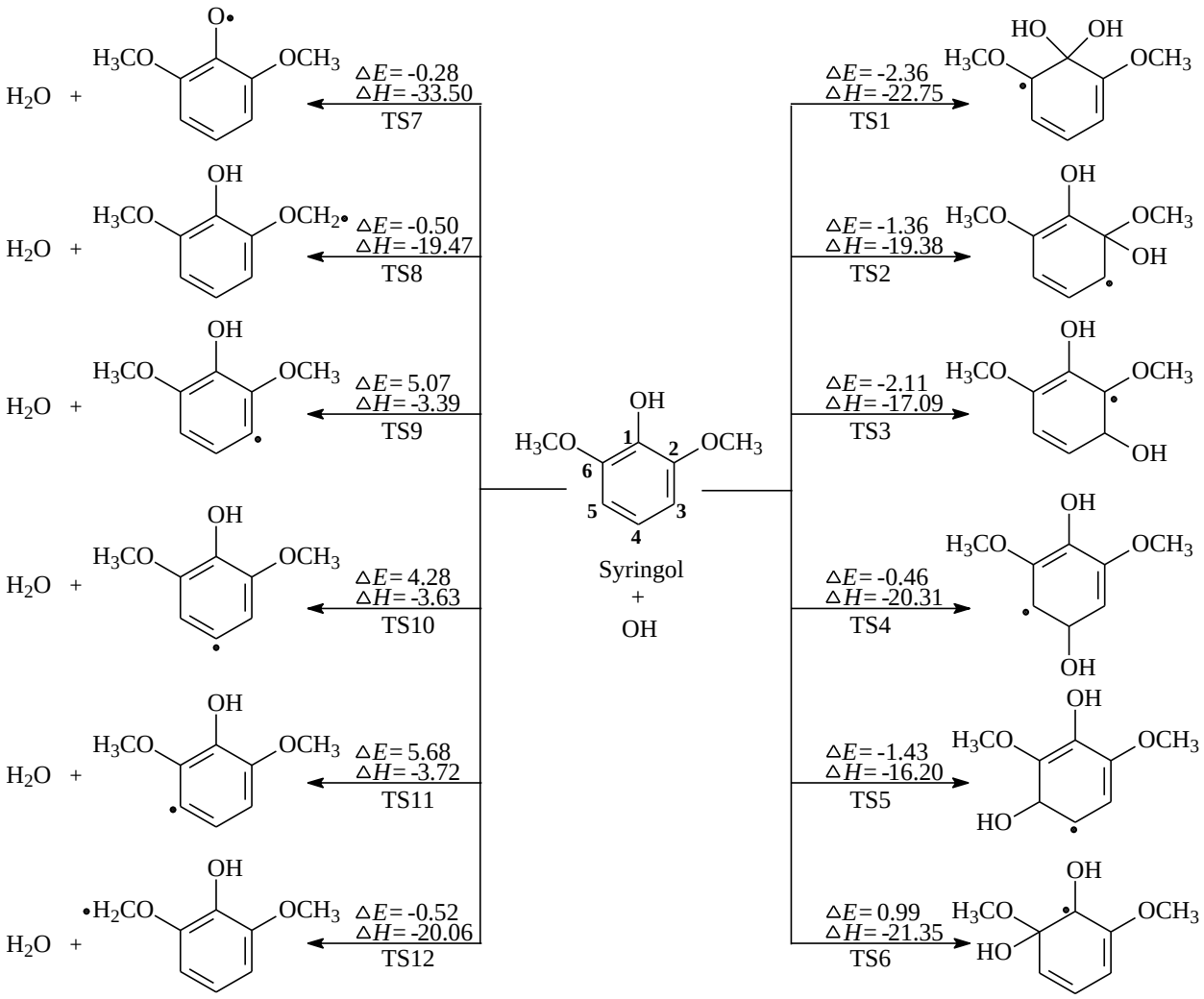


Figure S6. Profile of the potential energy surface for the reaction of creosol with OH radicals at the MPWB1K/6-311+G(3df,2p) level.

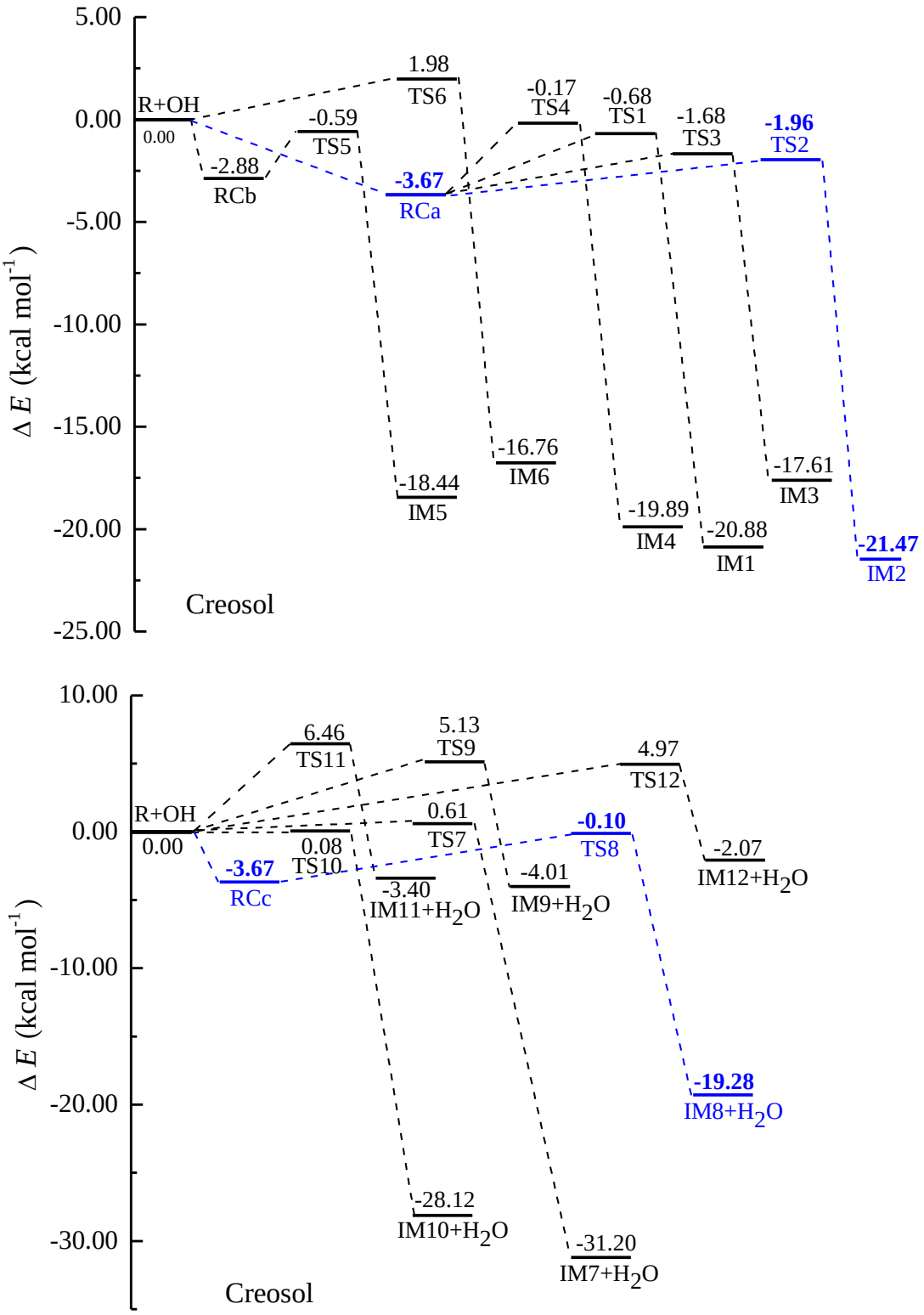


Figure S7. Profile of the potential energy surface for the reaction of syringol with OH radicals at the MPWB1K/6-311+G(3df,2p) level.

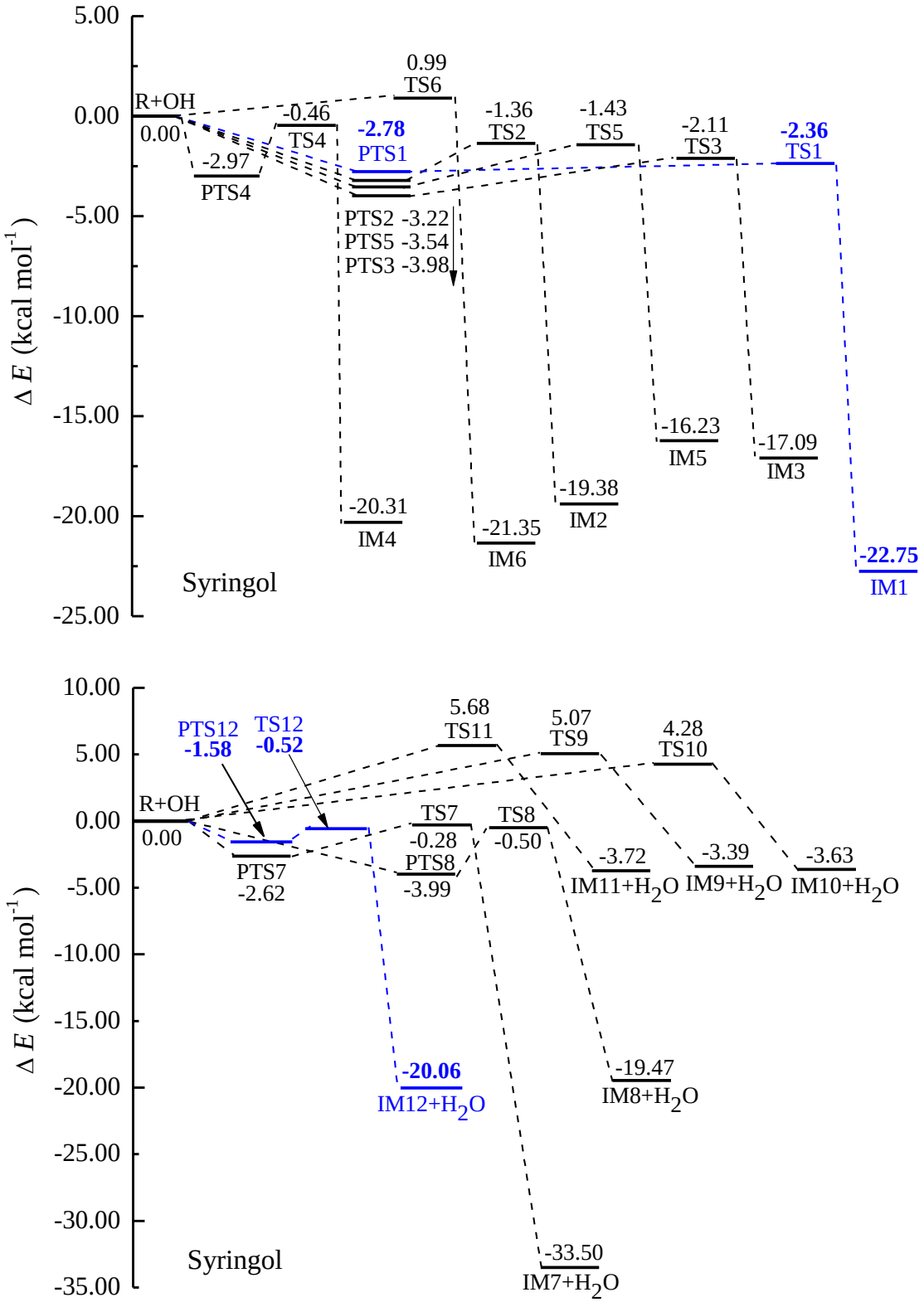


Figure S8. Secondary reaction scheme of IM2 with the potential barriers $\triangle E$ (kcal mol^{-1}) and reaction heats $\triangle H$ (kcal mol^{-1}).

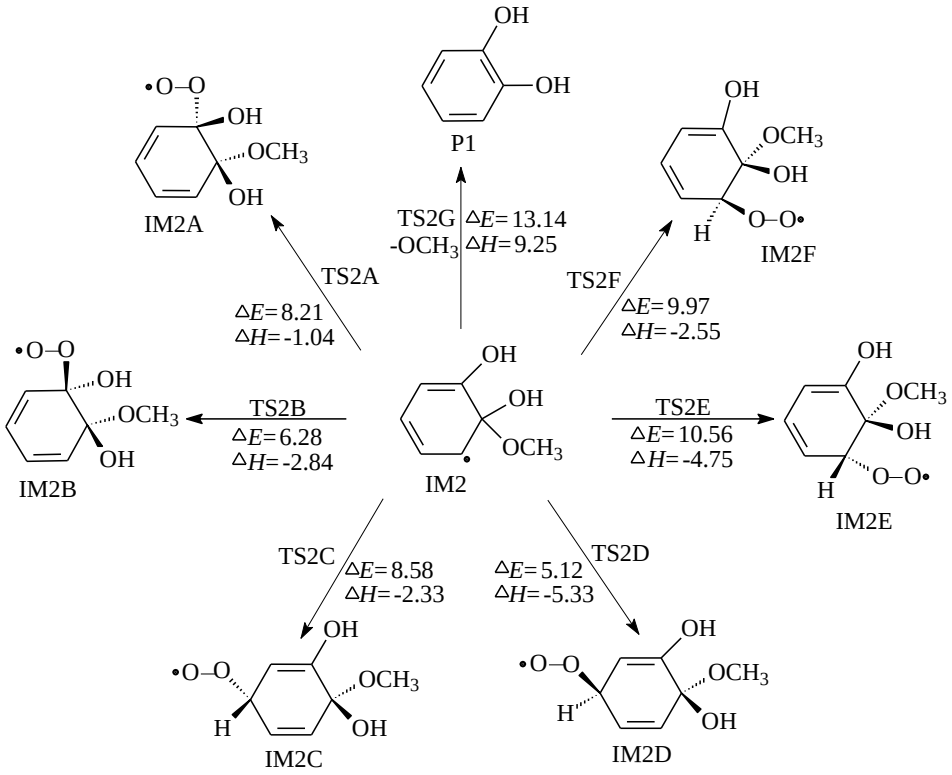


Figure S9. Secondary reaction scheme of IM2B-7 with the potential barriers $\triangle E$ (kcal mol^{-1}) and reaction heats $\triangle H$ (kcal mol^{-1}).

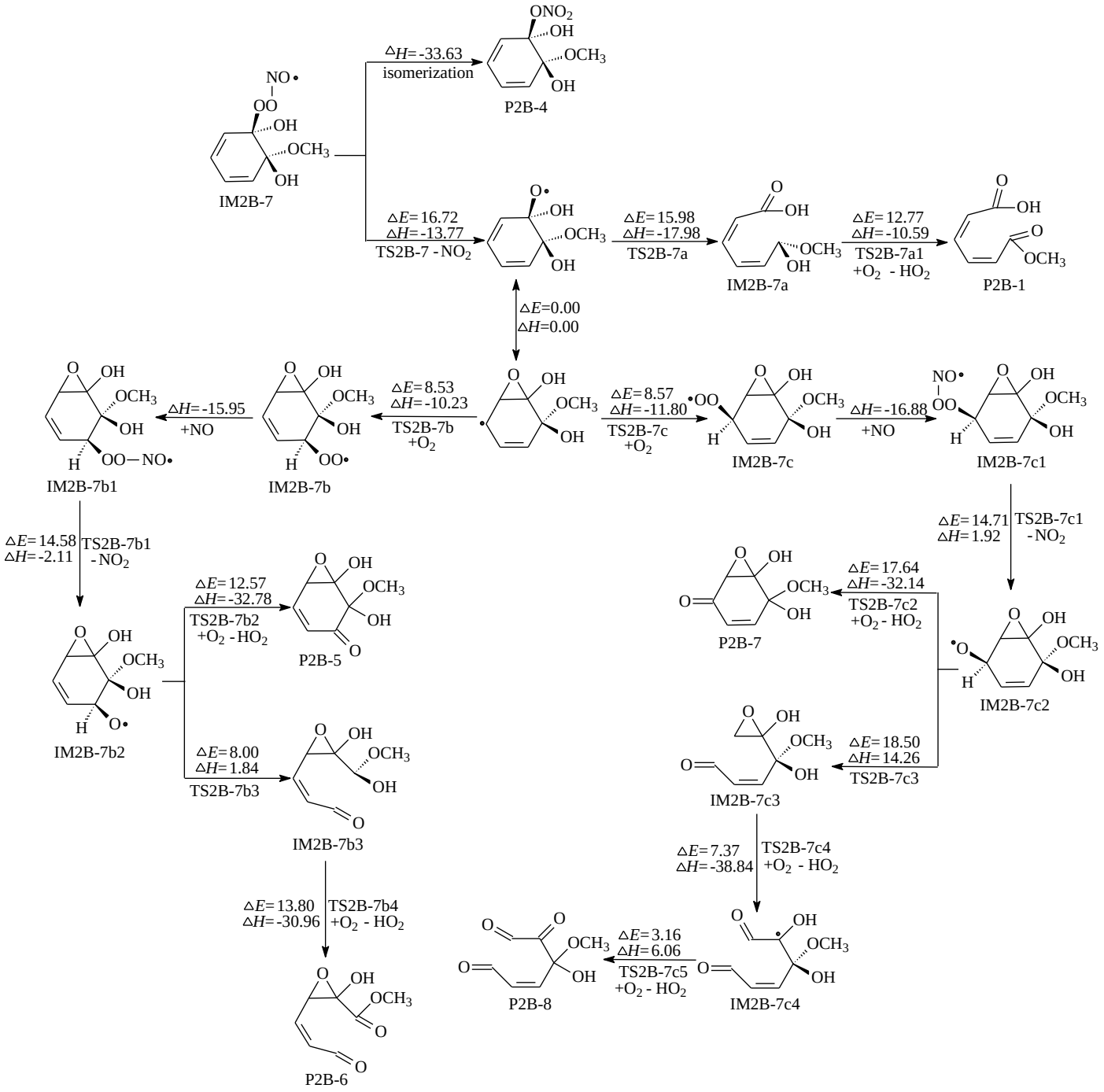


Figure S10. Secondary reaction scheme of IM2D with the potential barriers $\triangle E$ (kcal mol^{-1}) and reaction heats $\triangle H$ (kcal mol^{-1}).

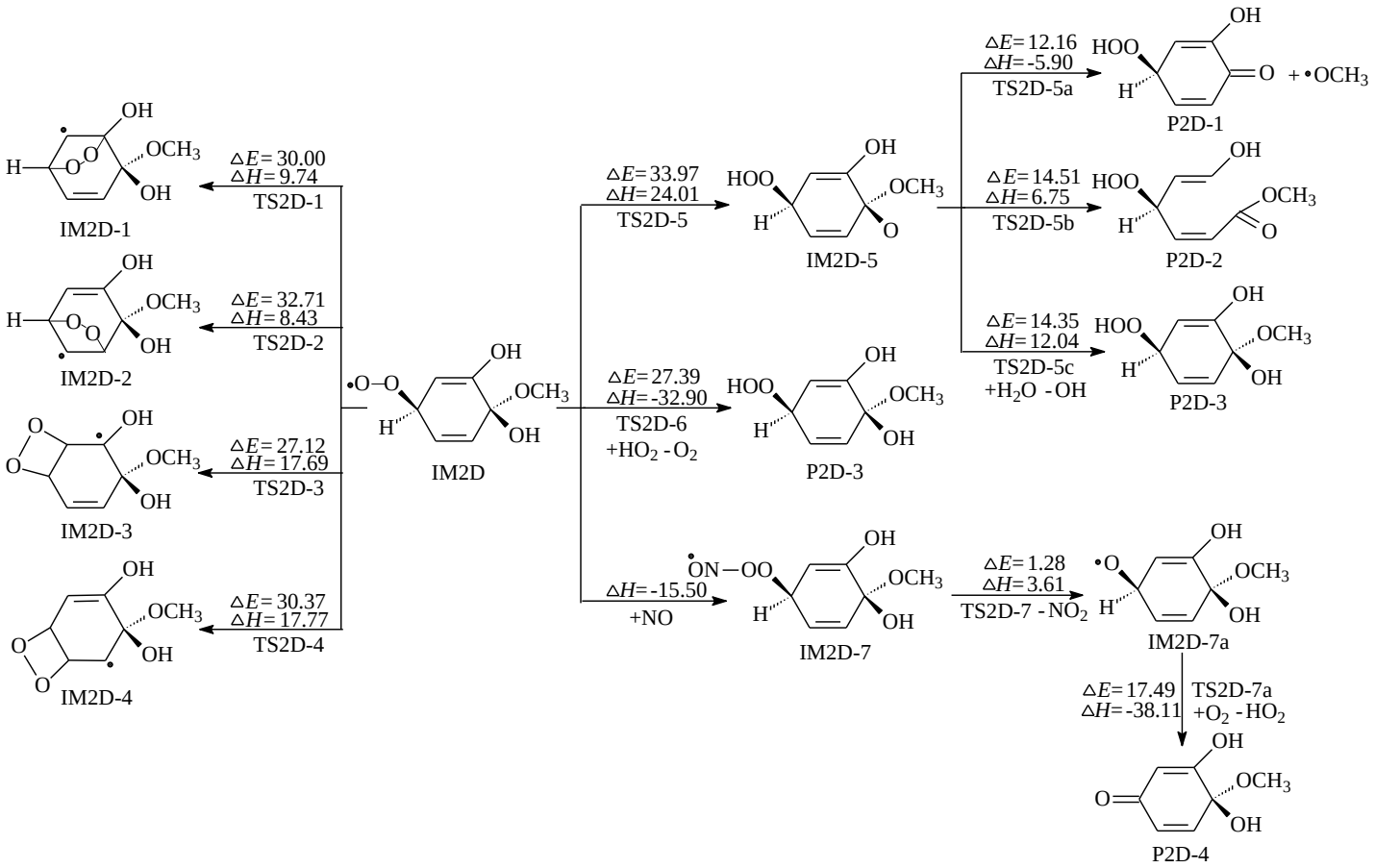
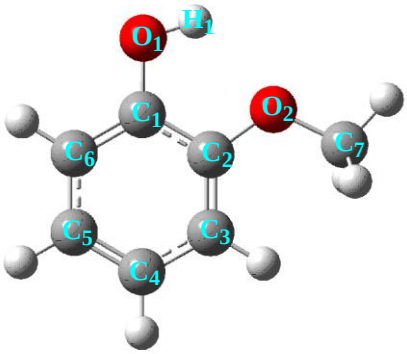


Table S1. The T1 diagnostic values of the key transition states involved in the initial reactions guaiacol with OH radicals at CCSD/6-311+G(d,p) level.

Species	T1 Diagnostic	Species	T1 Diagnostic
TS1	0.035	TS7	0.033
TS2	0.035	TS8	0.020
TS3	0.035	TS9	0.033
TS4	0.034	TS10	0.033
TS5	0.034	TS11	0.033
TS6	0.035	TS12	0.033

Table S2. The selected geometrical parameters of guaiacol obtained at MPWB1K, B3LYP and M06-2X methods along with 6-31+G(d,p) level. Bond lengths are in angstrom, and bond angles are in degree.



Parameter	MPWB1K	B3LYP	M06-2X
C1-C2	1.396	1.410	1.406
C2-C3	1.379	1.394	1.389
C3-C4	1.390	1.403	1.400
C4-C5	1.380	1.394	1.389
C5-C6	1.388	1.400	1.397
C6-C1	1.377	1.391	1.386
C1-O1	1.346	1.366	1.358
O1-H1	0.959	0.970	0.967
C2-O2	1.357	1.377	1.369
O2-C7	1.401	1.423	1.413
C1-O1-H1	108.2	108.0	108.3
C2-O2-C7	117.8	118.5	117.5

Table S3. Potential barriers ΔE (kcal mol^{-1}) and reaction heats ΔH (kcal mol^{-1}) for the initial reactions of guaiacol with OH radicals calculated at different levels of theory.

Reactions (Guaiacol + OH)	MPWB1K/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p)		CCSD(T)/6-311+G(d,p)//MPWB1K/6-31+G(d,p)		CCSD(T)/6-311+G(d,p)//B3LYP/6-31+G(d,p)		CCSD(T)/6-311+G(d,p)//M06-2X/6-31+G(d,p)	
	ΔE	*ΔH*	*ΔE*	*ΔH*	*ΔE*	*ΔH*	*ΔE*	*ΔH*
R+ OH → IM1	-0.20	-19.89	-0.20	-20.16	0.51	-20.20	0.50	-19.96
R + OH → IM2	-1.92	-20.81	-1.65	-20.89	-0.97	-20.90	-1.10	-20.76
R+ OH → IM3	-0.46	-16.17	0.63	-14.30	1.15	-14.40	1.07	-14.15
R + OH → IM4	-0.08	-18.76	1.67	-16.11	2.25	-16.33	2.03	-16.15
R + OH → IM5	1.19	-16.68	2.93	-13.77	3.38	-14.04	3.27	-13.67
R + OH → IM6	2.42	-16.03	3.31	-13.66	3.77	-13.95	3.84	-13.72
R + OH → IM7 + H_2O	0.99	-29.50	3.71	-27.83	3.35	-27.61	3.47	-27.64
R + OH → IM8 + H_2O	-0.10	-19.40	2.02	-18.17	2.50	-18.11	2.03	-18.17
R + OH → IM9 + H_2O	5.33	-4.17	7.41	-2.46	7.64	-2.04	7.82	-2.00
R + OH → IM10 + H_2O	4.53	-3.33	6.93	-1.36	5.76	-1.16	6.05	-1.00
R + OH → IM11 + H_2O	4.62	-3.36	7.09	-1.31	5.95	-1.19	6.10	-1.07
R + OH → IM12 + H_2O	4.68	-1.95	6.89	0.06	5.84	0.22	5.96	0.38

Table S4. The CPU times of some selected structures for reactions of guaiacol with OH radicals at MPWB1K/6-311+G(3df,2p) and CCSD(T)/6-311+G(d,p) level.

	MPWB1K/6-311+G(3df,2p)	CCSD(T)/6-311+G(d,p)
Guaiacol	38 minutes 30.1 seconds.	14 hours 15 minutes 54.9 seconds
IM5	1 hours 7 minutes 4.4 seconds	4 days 2 hours 53 minutes 31.1 seconds
IM6	1 hours 7 minutes 18.3 seconds	4 days 17 hours 42 minutes 47.1 seconds
TS2	1 hours 29 minutes 32.2 seconds	5 days 12 hours 9 minutes 56.9 seconds
TS3	1 hours 30 minutes 44.8 seconds	5 days 5 hours 34 minutes 39.5 seconds
TS4	1 hours 18 minutes 23.5 seconds	5 days 7 hours 54 minutes 12.9 seconds
TS5	1 hours 11 minutes 28.2 seconds	5 days 15 hours 43 minutes 31.9 seconds
TS6	1 hours 11 minutes 5.4 seconds	5 days 5 hours 58 minutes 48.9 seconds

Table S5. Rate constants k (cm^3 $molecule^{-1}$ s^{-1}) and branching ratio R for the reaction of creosol with OH radicals at 294 K and 1 atm.

Reactions	k_{294K}	R (%)
Creosol + OH → IM1	1.01×10^{-11}	12.95
Creosol + OH → IM2	2.96×10^{-11}	37.95
Creosol + OH → IM3	2.57×10^{-11}	32.95
Creosol + OH → IM4	2.00×10^{-12}	2.56
Creosol + OH → IM5	9.44×10^{-12}	12.10
Creosol + OH → IM6	1.18×10^{-15}	1.51e-3
Creosol + OH → IM7 + H_2O	9.73×10^{-14}	0.12
Creosol + OH → IM8 + H_2O	9.53×10^{-13}	1.22
Creosol + OH → IM9 + H_2O	2.03×10^{-18}	2.60e-6
Creosol + OH → IM10 + H_2O	1.13×10^{-13}	0.14
Creosol + OH → IM11 + H_2O	3.95×10^{-19}	5.06e-7
Creosol + OH → IM12 + H_2O	1.08×10^{-18}	1.38e-6
Creosol + OH → Products	7.80×10^{-11}	100

Table S6. Rate constants k (cm^3 $molecule^{-1}$ s^{-1}) and branching ratio R for the reaction of syringol with OH radicals at 294 K and 1 atm.

Reactions	k_{294K}	R (%)
Syringol + OH → IM1	2.53×10^{-11}	27.18
Syringol + OH → IM2	1.50×10^{-11}	16.11
Syringol + OH → IM3	2.11×10^{-11}	22.66
Syringol + OH → IM4	5.05×10^{-12}	5.42
Syringol + OH → IM5	1.43×10^{-11}	15.36
Syringol + OH → IM6	1.33×10^{-14}	0.01
Syringol + OH → IM7 + H_2O	3.11×10^{-12}	3.34
Syringol + OH → IM8 + H_2O	4.56×10^{-12}	4.90
Syringol + OH → IM9 + H_2O	9.51×10^{-18}	1.02e-5
Syringol + OH → IM10 + H_2O	1.74×10^{-17}	1.87e-5
Syringol + OH → IM11 + H_2O	4.39×10^{-18}	4.72e-6
Syringol + OH → IM12 + H_2O	4.67×10^{-12}	5.02
Syringol + OH → Products	9.31×10^{-11}	100

MESMER input files

Guaiacol + OH → IM1

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            <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
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z3="-0.889139" />
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      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
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Guaiacol + OH → IM2

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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805.93 859.94 929.77 991.83 1034.68 1035.53 1087.47 1142.23 1164.78 1179.59
1211.30 1231.93 1248.27 1304.55 1319.62 1359.95 1418.70 1479.56 1505.58
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</property>
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<array units="cm-1">0.089 0.053 0.033</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>
<molecule id="oh" spinMultiplicity="2">
<atomArray>
<atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.000000" z3="0.107474" />
<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
</atomArray>
<bondArray>
<bond atomRefs2="a2 a1" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>17.0073</scalar>
</property>

```
            <property title="Energy" dictRef="me:ZPE">
              <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
              <scalar>2.00</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
              <array units="cm-1">3870.53</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
              <array units="cm-1">18.991</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
              <scalar>1</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
              <scalar>1</scalar>
            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
      </moleculeList>
      <reactionList>
        <reaction id="r1" reversible="true">
          <reactantList>
            <reactant>
              <molecule ref="R1b" role="deficientReactant" />
            </reactant>
            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM2" role="modelled" />
            </product>
          </productList>
          <rateParameters reactionType="arrhenius" reversible="true">
            <A>3.5000e-011</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
          <me:MCRCMethod default="true" DefinedSumOfStates,
```

```
LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
        <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true"
bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
```

```
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_222013</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Guaiacol + OH → IM3

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190902_144100" />
    </molecule>
    <molecule id="IM3" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.352368" y3="0.258574"
z3="-0.064657" />
        <atom id="a2" elementType="C" x3="0.150781" y3="-1.206669"
z3="-0.223371" />
        <atom id="a3" elementType="C" x3="-1.288394" y3="-1.560854"
z3="-0.356056" />
        <atom id="a4" elementType="C" x3="-2.276070" y3="-0.644960"
z3="-0.235295" />
        <atom id="a5" elementType="C" spinMultiplicity="2" x3="-2.002137"
y3="0.723989" z3="-0.020227" />
        <atom id="a6" elementType="C" x3="-0.679390" y3="1.150853"
z3="0.064172" />
        <atom id="a7" elementType="H" x3="0.697601" y3="-1.561991"
z3="-1.101401" />
```

<atom id="a8" elementType="H" x3="-1.507524" y3="-2.604877" z3="-0.517580" />
<atom id="a9" elementType="O" x3="-0.424325" y3="2.460233" z3="0.269364" />
<atom id="a10" elementType="H" x3="0.527373" y3="2.574763" z3="0.294035" />
<atom id="a11" elementType="H" x3="-3.305849" y3="-0.960480" z3="-0.308871" />
<atom id="a12" elementType="H" x3="-2.792135" y3="1.449537" z3="0.078026" />
<atom id="a13" elementType="O" x3="1.593002" y3="0.776650" z3="0.070060" />
<atom id="a14" elementType="C" x3="2.684827" y3="0.057727" z3="-0.459754" />
<atom id="a15" elementType="H" x3="2.589102" y3="-0.043491" z3="-1.540200" />
<atom id="a16" elementType="H" x3="3.566684" y3="0.644986" z3="-0.234655" />
<atom id="a17" elementType="H" x3="2.765154" y3="-0.921021" z3="0.004166" />
<atom id="a18" elementType="O" x3="0.772746" y3="-1.924570" z3="0.842551" />
<atom id="a19" elementType="H" x3="0.276315" y3="-1.747888" z3="1.641805" />
</atomArray>
<bondArray>
<bond atomRefs2="a15 a14" order="1" />
<bond atomRefs2="a7 a2" order="1" />
<bond atomRefs2="a8 a3" order="1" />
<bond atomRefs2="a14 a16" order="1" />
<bond atomRefs2="a14 a17" order="1" />
<bond atomRefs2="a14 a13" order="1" />
<bond atomRefs2="a3 a4" order="2" />
<bond atomRefs2="a3 a2" order="1" />
<bond atomRefs2="a11 a4" order="1" />
<bond atomRefs2="a4 a5" order="1" />
<bond atomRefs2="a2 a1" order="1" />
<bond atomRefs2="a2 a18" order="1" />
<bond atomRefs2="a1 a6" order="2" />
<bond atomRefs2="a1 a13" order="1" />
<bond atomRefs2="a5 a6" order="1" />
<bond atomRefs2="a5 a12" order="1" />
<bond atomRefs2="a6 a9" order="1" />
<bond atomRefs2="a9 a10" order="1" />

```
      <bond atomRefs2="a18 a19" order="1" />
    </bondArray>
    <propertyList>
      <property title="program">
        <scalar>Gaussian 09, Revision B.01</scalar>
      </property>
      <property title="basis">
        <scalar>6-31+G(d,p) (6D, 7F)</scalar>
      </property>
      <property title="method">
        <scalar>umpwb95</scalar>
      </property>
      <property title="File Format">
        <scalar>g03</scalar>
      </property>
      <property title="MW">
        <scalar>141.145</scalar>
      </property>
      <property title="Energy" dictRef="me:ZPE">
        <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">-16.17</scalar>
      </property>
      <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
        <scalar>2.00</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">84.00 114.18 190.08 204.40 239.13 278.51 324.75
347.79 395.76 455.87 481.03 493.85 527.40 567.54 583.26 657.32 729.21 770.56
812.19 849.54 993.11 1008.01 1058.74 1089.71 1115.41 1195.04 1202.93 1211.05
1239.28 1244.66 1297.52 1335.46 1358.99 1420.20 1427.63 1459.70 1482.53
1523.70 1533.47 1571.16 1642.59 1675.32 3083.94 3112.85 3207.26 3249.77
3270.64 3291.20 3310.06 3932.40 3950.62</array>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
        <array units="cm-1">0.058 0.048 0.029</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:sigma" default="true">
        <scalar>5.0</scalar>
      </property>
      <property dictRef="me:epsilon" default="true">
        <scalar>50.0</scalar>
```

```
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
      <molecule id="R1b" spinMultiplicity="1" default="true">
         <atomArray>
            <atom id="a1" elementType="C" x3="0.438888" y3="-0.074767"
z3="0.000093" />
            <atom id="a2" elementType="C" x3="-0.008362" y3="-1.379710"
z3="0.000077" />
            <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
z3="0.000036" />
            <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
z3="-0.000055" />
            <atom id="a5" elementType="C" x3="-1.823901" y3="0.722310"
z3="-0.000072" />
            <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
z3="0.000041" />
            <atom id="a7" elementType="H" x3="0.693038" y3="-2.198155"
z3="0.000160" />
            <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
z3="-0.000061" />
            <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
z3="0.000074" />
            <atom id="a10" elementType="H" x3="0.936931" y3="2.229396"
z3="-0.000245" />
            <atom id="a11" elementType="H" x3="-3.335842" y3="-0.786514"
z3="-0.000161" />
            <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
            <atom id="a13" elementType="O" x3="1.738049" y3="0.317486"
z3="-0.000027" />
            <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
            <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
z3="-0.889139" />
            <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
z3="-0.000547" />
```

```
            <atom id="a17" elementType="H" x3="2.645011" y3="-1.304143"
z3="0.889410" />
         </atomArray>
         <bondArray>
            <bond atomRefs2="a15 a14" order="1" />
            <bond atomRefs2="a16 a14" order="1" />
            <bond atomRefs2="a10 a9" order="1" />
            <bond atomRefs2="a11 a4" order="1" />
            <bond atomRefs2="a12 a5" order="1" />
            <bond atomRefs2="a5 a4" order="2" />
            <bond atomRefs2="a5 a6" order="1" />
            <bond atomRefs2="a14 a13" order="1" />
            <bond atomRefs2="a14 a17" order="1" />
            <bond atomRefs2="a8 a3" order="1" />
            <bond atomRefs2="a4 a3" order="1" />
            <bond atomRefs2="a13 a1" order="1" />
            <bond atomRefs2="a3 a2" order="2" />
            <bond atomRefs2="a6 a9" order="1" />
            <bond atomRefs2="a6 a1" order="2" />
            <bond atomRefs2="a2 a1" order="1" />
            <bond atomRefs2="a2 a7" order="1" />
         </bondArray>
         <propertyList>
            <property title="program">
               <scalar>Gaussian 09, Revision B.01</scalar>
            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
            <property title="method">
               <scalar>umpwb95</scalar>
            </property>
            <property title="File Format">
               <scalar>g03</scalar>
            </property>
            <property title="MW">
               <scalar>124.137</scalar>
            </property>
            <property title="Energy" dictRef="me:ZPE">
               <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
               <array units="cm-1">82.23 191.53 245.13 283.01 332.55 359.31 459.66
```

480.40 517.10 552.95 589.56 602.06 737.96 777.62 803.74 868.03 880.89 960.92 1007.99 1085.06 1118.79 1169.09 1201.41 1205.10 1236.53 1263.04 1322.64 1352.43 1366.37 1448.85 1514.85 1533.78 1544.67 1553.14 1604.13 1721.73 1733.25 3100.95 3176.46 3245.64 3276.82 3289.07 3298.07 3304.40 3932.57</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.089 0.053 0.033</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>
<molecule id="oh" spinMultiplicity="2">
<atomArray>
<atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.000000" z3="0.107474" />
<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
</atomArray>
<bondArray>
<bond atomRefs2="a2 a1" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>17.0073</scalar>
</property>

```
            <property title="Energy" dictRef="me:ZPE">
              <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
              <scalar>2.00</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
              <array units="cm-1">3870.53</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
              <array units="cm-1">18.991</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
              <scalar>1</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
              <scalar>1</scalar>
            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
      </moleculeList>
      <reactionList>
        <reaction id="r1" reversible="true">
          <reactantList>
            <reactant>
              <molecule ref="R1b" role="deficientReactant" />
            </reactant>
            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM3" role="modelled" />
            </product>
          </productList>
          <rateParameters reactionType="arrhenius" reversible="true">
            <A>1.500e-011</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
          <me:MCRCMethod default="true DefinedSumOfStates,
```

```
LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
          <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
          <me:TInfinity default="true">298</me:TInfinity>
        </reaction>
    </reactionList>
    <me:conditions>
        <me:bathGas>He</me:bathGas>
        <me:PTs>
          <me:PTpair units="Torr" P="760" T="294." precision="d" default="true"
bathGas="He" />
          <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
          <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
          <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
        </me:PTs>
    </me:conditions>
    <me:modelParameters>
        <!--Specify grain size directly...-->
        <me:grainSize units="cm-1">100</me:grainSize>
        <!--...or by the total number of grains
              <me:numberOfGrains> 500 </me:numberOfGrains>-->
        <!--Specify increased energy range
              <me:maxTemperature>6000</me:maxTemperature>-->
        <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
        <me:testDOS />
        <me:printSpeciesProfile />
        <!--<me:testMicroRates />-->
        <me:testRateConstant />
        <me:printGrainDOS />
        <!--<me:printCellDOS />-->
        <!--<me:printReactionOperatorColumnSums />-->
        <!--<me:printTunnellingCoefficients />-->
        <me:printGrainkfE />
        <!--<me:printGrainBoltzmann />-->
        <me:printGrainkbE />
        <me:eigenvalues>0</me:eigenvalues>
        <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
        <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
        <!--Adjusts displayed energies to this values for the lowest species. -->
        <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
```

```
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_222116</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Guaiacol + OH → IM4

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190902_203143" />
    </molecule>
    <molecule id="IM4" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.685060" y3="-0.109347"
z3="-0.075520" />
        <atom id="a2" elementType="C" x3="-0.260079" y3="-1.048157"
z3="-0.288307" />
        <atom id="a3" elementType="C" x3="-1.707209" y3="-0.700860"
z3="-0.378105" />
        <atom id="a4" elementType="C" spinMultiplicity="2" x3="-1.964694"
y3="0.764842" z3="-0.295557" />
        <atom id="a5" elementType="C" x3="-0.980924" y3="1.674807"
z3="-0.081580" />
        <atom id="a6" elementType="C" x3="0.352723" y3="1.270361"
z3="0.029423" />
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      </property>
      <property title="basis">
        <scalar>6-31+G(d,p) (6D, 7F)</scalar>
      </property>
      <property title="method">
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      <property title="File Format">
        <scalar>g03</scalar>
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        <scalar>141.145</scalar>
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zeroPointVibEnergyAdded="true">-18.76</scalar>
      </property>
      <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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347.61 387.95 438.60 473.40 505.05 536.01 557.55 608.94 655.72 755.93 783.27
813.44 845.11 945.23 974.28 1059.19 1105.14 1127.72 1186.97 1205.90 1219.32
1242.91 1254.75 1316.56 1362.01 1373.55 1405.98 1430.64 1465.11 1511.11
1526.57 1544.06 1561.28 1633.72 1720.54 3092.76 3106.23 3183.62 3249.09
3278.82 3295.39 3306.81 3907.39 3953.68</array>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
        <array units="cm-1">0.063 0.039 0.025</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:sigma" default="true">
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         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
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z3="0.000093" />
            <atom id="a2" elementType="C" x3="-0.008362" y3="-1.379710"
z3="0.000077" />
            <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
z3="0.000036" />
            <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
z3="-0.000055" />
            <atom id="a5" elementType="C" x3="-1.823901" y3="0.722310"
z3="-0.000072" />
            <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
z3="0.000041" />
            <atom id="a7" elementType="H" x3="0.693038" y3="-2.198155"
z3="0.000160" />
            <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
z3="-0.000061" />
            <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
z3="0.000074" />
            <atom id="a10" elementType="H" x3="0.936931" y3="2.229396"
z3="-0.000245" />
            <atom id="a11" elementType="H" x3="-3.335842" y3="-0.786514"
z3="-0.000161" />
            <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
            <atom id="a13" elementType="O" x3="1.738049" y3="0.317486"
z3="-0.000027" />
            <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
            <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
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            <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
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</property>
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480.40 517.10 552.95 589.56 602.06 737.96 777.62 803.74 868.03 880.89 960.92 1007.99 1085.06 1118.79 1169.09 1201.41 1205.10 1236.53 1263.04 1322.64 1352.43 1366.37 1448.85 1514.85 1533.78 1544.67 1553.14 1604.13 1721.73 1733.25 3100.95 3176.46 3245.64 3276.82 3289.07 3298.07 3304.40 3932.57</array>
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<property dictRef="me:frequenciesScaleFactor" default="true">
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</property>
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      </moleculeList>
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            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM4" role="modelled" />
            </product>
          </productList>
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            <A>5.000e-012</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
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LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
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        <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
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    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
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bathGas="He" />
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        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
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    </me:conditions>
    <me:modelParameters>
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      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_222249</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
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Guaiacol + OH → IM5

```
<?xml version="1.0" encoding="utf-8" ?>
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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
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timestamp="20190908_141402" />
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z3="-0.149844" />
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y3="-1.436219" z3="-0.309893" />
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z3="-0.255111" />
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```
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            <atom id="a10" elementType="H" x3="1.626143" y3="2.112782"
z3="0.113590" />
            <atom id="a11" elementType="H" x3="-2.599302" y3="-0.267565"
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z3="0.112873" />
            <atom id="a14" elementType="C" x3="3.014384" y3="-0.976960"
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            <atom id="a15" elementType="H" x3="2.963640" y3="-1.556308"
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            <atom id="a16" elementType="H" x3="4.014075" y3="-0.579805"
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            <atom id="a17" elementType="H" x3="2.769935" y3="-1.614878"
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      </property>
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346.81 390.64 411.38 437.74 480.70 513.67 584.10 601.10 649.88 744.05 768.12
809.69 858.08 939.72 953.04 1057.27 1102.27 1137.49 1202.46 1203.71 1234.15
1239.60 1262.79 1286.40 1337.08 1369.95 1396.56 1423.90 1466.79 1513.61
1534.12 1544.90 1558.29 1615.90 1730.46 3081.39 3108.90 3188.29 3251.33
3280.20 3294.18 3297.86 3940.24 3954.77</array>
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         <me:deltaEDown default="true">250.0</me:deltaEDown>
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z3="0.000077" />
            <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
z3="0.000036" />
            <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
z3="-0.000055" />
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</property>
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812.70 875.59 891.11 957.99 1014.38 1056.85 1118.07 1162.44 1204.69 1208.50
1232.81 1267.93 1319.96 1355.56 1374.69 1438.29 1511.41 1530.09 1531.61
1546.64 1601.27 1655.17 1712.06 3108.90 3188.18 3253.13 3297.44 3305.55
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    <me:modelParameters>
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
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    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
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      <me:testRateConstant />
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      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
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Guaiacol + OH → IM6

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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819.21 840.36 978.48 994.44 1073.82 1114.14 1129.45 1205.16 1208.61 1223.83
1233.30 1245.48 1287.32 1351.93 1361.85 1405.25 1455.20 1479.07 1507.56
1516.74 1536.14 1551.36 1650.77 1693.77 2991.77 3102.21 3178.50 3242.65
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480.40 517.10 552.95 589.56 602.06 737.96 777.62 803.74 868.03 880.89 960.92 1007.99 1085.06 1118.79 1169.09 1201.41 1205.10 1236.53 1263.04 1322.64 1352.43 1366.37 1448.85 1514.85 1533.78 1544.67 1553.14 1604.13 1721.73 1733.25 3100.95 3176.46 3245.64 3276.82 3289.07 3298.07 3304.40 3932.57</array>
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324.51 356.29 463.94 512.30 520.87 550.89 570.42 596.70 723.67 778.27 798.35
825.85 862.93 893.79 975.28 1007.65 1078.17 1112.84 1159.53 1206.90 1210.26
1230.30 1257.91 1318.92 1357.20 1368.33 1460.52 1511.00 1519.54 1533.77
1551.97 1591.76 1687.25 1699.34 3103.62 3180.63 3249.01 3281.77 3299.29
3304.72 3311.28 3896.67 3907.04</array>
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y3="0.000000" z3="0.107474" />
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z3="-0.859789" />
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            <molecule ref="oh" role="excessReactant" />
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        </productList>
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        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
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        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
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    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
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      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
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      <dc:date>20190908_192436</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
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Guaiacol + OH → IM7 + H_2O

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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  <moleculeList convention="">
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        <property dictRef="me:sigma">
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</property>

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z3="0.000036" />
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</property>
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</property>
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<scalar>141.145</scalar>
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</cml>

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309.02 349.90 370.35 480.86 519.74 549.78 578.89 604.18 672.84 753.92 783.97
809.34 881.57 882.63 972.13 1012.14 1097.02 1123.96 1175.67 1203.95 1208.51
1243.54 1272.21 1338.02 1372.91 1384.75 1430.94 1511.58 1536.61 1541.61
1555.69 1568.42 1681.80 1712.90 2219.66 3101.91 3179.20 3252.80 3277.30
3290.25 3301.57 3307.03 3917.83</array>
            </property>
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z3="-0.859789" />
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            </property>
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            </property>
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               <scalar>17.0073</scalar>
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            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
               <array units="cm-1">3870.53</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
               <array units="cm-1">18.991</array>
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            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
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            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
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   </moleculeList>
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            </reactant>
            <reactant>
               <molecule ref="oh" role="excessReactant" />
            </reactant>
         </reactantList>
         <productList>
            <product>
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        </me:transitionState>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
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```
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_211836</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
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Guaiacol + OH → IM8 + H_2O

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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        <atom elementType="He" />
      </atomArray>
      <propertyList>
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          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
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timestamp="20190903_103712" />
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z3="-0.093439" />
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        <atom id="a3" elementType="C" x3="-1.453556" y3="-1.559986"
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        <atom id="a4" elementType="C" x3="-2.265910" y3="-0.444661"
z3="0.067929" />
        <atom id="a5" elementType="C" x3="-1.715985" y3="0.826940"
z3="0.079862" />
        <atom id="a6" elementType="C" x3="-0.347496" y3="0.985617"
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<atom id="a10" elementType="H" x3="1.143185" y3="2.137310" z3="-0.050959" />
<atom id="a11" elementType="H" x3="-3.336344" y3="-0.560311" z3="0.132727" />
<atom id="a12" elementType="H" x3="-2.333178" y3="1.707757" z3="0.155874" />
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<atom id="a14" elementType="C" spinMultiplicity="2" x3="2.696813" y3="-0.807180" z3="0.171466" />
<atom id="a15" elementType="H" x3="3.713824" y3="-0.485790" z3="0.039005" />
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<bond atomRefs2="a2 a3" order="1" />
<bond atomRefs2="a1 a6" order="1" />
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<bond atomRefs2="a10 a9" order="1" />
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</property>

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<me:deltaEDown default="true">250.0</me:deltaEDown>
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z3="0.000077" />
    <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
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    <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
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    <atom id="a5" elementType="C" x3="-1.823901" y3="0.722310"
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    <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
z3="0.000041" />
    <atom id="a7" elementType="H" x3="0.693038" y3="-2.198155"
z3="0.000160" />
    <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
z3="-0.000061" />
    <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
z3="0.000074" />
    <atom id="a10" elementType="H" x3="0.936931" y3="2.229396"
z3="-0.000245" />
    <atom id="a11" elementType="H" x3="-3.335842" y3="-0.786514"
z3="-0.000161" />
    <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
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    <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
    <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
z3="-0.889139" />
    <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
z3="-0.000547" />
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z3="0.889410" />
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    <bond atomRefs2="a11 a4" order="1" />
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</property>
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          <atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
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          </property>
```

```
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            </property>
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      </moleculeList>
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              <molecule ref="oh" role="deficientReactant" />
            </reactant>
          </reactantList>
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            <product>
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            </product>
          </productList>
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            <n>0</n>
            <E>0</E>
          </rateParameters>
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          <me:TInfinity default="true">298</me:TInfinity>
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      </reactionList>
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```
bathGas="He" />
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        </me:PTs>
    </me:conditions>
    <me:modelParameters>
        <!--Specify grain size directly...-->
        <me:grainSize units="cm-1">100</me:grainSize>
        <!--...or by the total number of grains
              <me:numberOfGrains> 500 </me:numberOfGrains>-->
        <!--Specify increased energy range
              <me:maxTemperature>6000</me:maxTemperature>-->
        <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
        <me:testDOS />
        <me:printSpeciesProfile />
        <!--<me:testMicroRates />-->
        <me:testRateConstant />
        <me:printGrainDOS />
        <!--<me:printCellDOS />-->
        <!--<me:printReactionOperatorColumnSums />-->
        <!--<me:printTunnellingCoefficients />-->
        <me:printGrainkfE />
        <!--<me:printGrainBoltzmann />-->
        <me:printGrainkbE />
        <me:eigenvalues>0</me:eigenvalues>
        <!-- <me:hideInactive/>   Molecules and reactions with attribute active="false"
are not shown-->
        <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
        <!--Adjusts displayed energies to this values for the lowest species. -->
        <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
        <dc:title>Project name</dc:title>
        <dc:source>bve.xml</dc:source>
        <dc:creator>Mesmer v5.0</dc:creator>
        <dc:date>20190908_222532</dc:date>
        <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Guaiacol + OH → IM9 + H_2O

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190902_161522" />
    </molecule>
    <molecule id="IM9" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.472733" y3="-0.083723"
z3="-0.000002" />
        <atom id="a2" elementType="C" spinMultiplicity="2" x3="-0.034254"
y3="-1.350708" z3="0.000043" />
        <atom id="a3" elementType="C" x3="-1.363369" y3="-1.678983"
z3="0.000061" />
        <atom id="a4" elementType="C" x3="-2.257713" y3="-0.615820"
z3="0.000034" />
        <atom id="a5" elementType="C" x3="-1.802946" y3="0.694981"
z3="-0.000007" />
        <atom id="a6" elementType="C" x3="-0.449157" y3="0.968558"
z3="-0.000021" />
        <atom id="a7" elementType="H" x3="-1.703093" y3="-2.702400"
z3="0.000097" />
```

```
            <atom id="a8" elementType="O" x3="-0.006617" y3="2.238488"
z3="-0.000050" />
            <atom id="a9" elementType="H" x3="0.952361" y3="2.225388"
z3="-0.000136" />
            <atom id="a10" elementType="H" x3="-3.319199" y3="-0.810767"
z3="0.000044" />
            <atom id="a11" elementType="H" x3="-2.492307" y3="1.523714"
z3="-0.000029" />
            <atom id="a12" elementType="O" x3="1.776589" y3="0.270406"
z3="-0.000010" />
            <atom id="a13" elementType="C" x3="2.697565" y3="-0.791490"
z3="-0.000015" />
            <atom id="a14" elementType="H" x3="2.570340" y3="-1.409243"
z3="-0.887641" />
            <atom id="a15" elementType="H" x3="3.684442" y3="-0.345640"
z3="-0.000155" />
            <atom id="a16" elementType="H" x3="2.570526" y3="-1.409093"
z3="0.887743" />
         </atomArray>
         <bondArray>
            <bond atomRefs2="a14 a13" order="1" />
            <bond atomRefs2="a15 a13" order="1" />
            <bond atomRefs2="a9 a8" order="1" />
            <bond atomRefs2="a8 a6" order="1" />
            <bond atomRefs2="a11 a5" order="1" />
            <bond atomRefs2="a6 a5" order="2" />
            <bond atomRefs2="a6 a1" order="1" />
            <bond atomRefs2="a13 a12" order="1" />
            <bond atomRefs2="a13 a16" order="1" />
            <bond atomRefs2="a12 a1" order="1" />
            <bond atomRefs2="a5 a4" order="1" />
            <bond atomRefs2="a1 a2" order="2" />
            <bond atomRefs2="a4 a10" order="1" />
            <bond atomRefs2="a4 a3" order="2" />
            <bond atomRefs2="a2 a3" order="1" />
            <bond atomRefs2="a3 a7" order="1" />
         </bondArray>
         <propertyList>
            <property title="program">
               <scalar>Gaussian 09, Revision B.01</scalar>
            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
```

<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>123.129</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">-4.17</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">78.80 160.14 195.43 209.61 302.47 334.64 453.44 490.19 508.44 549.92 566.58 606.32 705.70 754.33 811.54 848.02 903.46 989.76 1083.59 1120.41 1174.99 1204.22 1204.34 1228.19 1286.67 1321.26 1361.97 1425.94 1495.86 1517.30 1521.47 1535.90 1587.85 1669.77 1731.06 3107.16 3182.67 3248.51 3274.83 3291.94 3303.93 3929.44</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.090 0.053 0.034</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:sigma" default="true">
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</property>
<property dictRef="me:epsilon" default="true">
<scalar>50.0</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
<me:DistributionCalcMethod default="true" name="Boltzmann" />
<me:energyTransferModel name="ExponentialDown" default="true" />
<me:deltaEDown default="true">250.0</me:deltaEDown>
</molecule>

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  <atomArray>
    <atom id="a1" elementType="C" x3="0.438888" y3="-0.074767"
z3="0.000093" />
    <atom id="a2" elementType="C" x3="-0.008362" y3="-1.379710"
z3="0.000077" />
    <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
z3="0.000036" />
    <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
z3="-0.000055" />
    <atom id="a5" elementType="C" x3="-1.823901" y3="0.722310"
z3="-0.000072" />
    <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
z3="0.000041" />
    <atom id="a7" elementType="H" x3="0.693038" y3="-2.198155"
z3="0.000160" />
    <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
z3="-0.000061" />
    <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
z3="0.000074" />
    <atom id="a10" elementType="H" x3="0.936931" y3="2.229396"
z3="-0.000245" />
    <atom id="a11" elementType="H" x3="-3.335842" y3="-0.786514"
z3="-0.000161" />
    <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
    <atom id="a13" elementType="O" x3="1.738049" y3="0.317486"
z3="-0.000027" />
    <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
    <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
z3="-0.889139" />
    <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
z3="-0.000547" />
    <atom id="a17" elementType="H" x3="2.645011" y3="-1.304143"
z3="0.889410" />
  </atomArray>
  <bondArray>
    <bond atomRefs2="a15 a14" order="1" />
    <bond atomRefs2="a16 a14" order="1" />
    <bond atomRefs2="a10 a9" order="1" />
    <bond atomRefs2="a11 a4" order="1" />
    <bond atomRefs2="a12 a5" order="1" />
    <bond atomRefs2="a5 a4" order="2" />
```

<bond atomRefs2="a5 a6" order="1" />
<bond atomRefs2="a14 a13" order="1" />
<bond atomRefs2="a14 a17" order="1" />
<bond atomRefs2="a8 a3" order="1" />
<bond atomRefs2="a4 a3" order="1" />
<bond atomRefs2="a13 a1" order="1" />
<bond atomRefs2="a3 a2" order="2" />
<bond atomRefs2="a6 a9" order="1" />
<bond atomRefs2="a6 a1" order="2" />
<bond atomRefs2="a2 a1" order="1" />
<bond atomRefs2="a2 a7" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>124.137</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">82.23 191.53 245.13 283.01 332.55 359.31 459.66 480.40 517.10 552.95 589.56 602.06 737.96 777.62 803.74 868.03 880.89 960.92 1007.99 1085.06 1118.79 1169.09 1201.41 1205.10 1236.53 1263.04 1322.64 1352.43 1366.37 1448.85 1514.85 1533.78 1544.67 1553.14 1604.13 1721.73 1733.25 3100.95 3176.46 3245.64 3276.82 3289.07 3298.07 3304.40 3932.57</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.089 0.053 0.033</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>
<molecule id="TS9" spinMultiplicity="2">
<atomArray>
<atom id="a1" elementType="C" x3="0.459926" y3="-0.081874" z3="-0.022864" />
<atom id="a2" elementType="C" spinMultiplicity="2" x3="-0.023348" y3="-1.368966" z3="0.034450" />
<atom id="a3" elementType="C" x3="-1.374485" y3="-1.654796" z3="0.064951" />
<atom id="a4" elementType="C" x3="-2.273003" y3="-0.603875" z3="0.045911" />
<atom id="a5" elementType="C" x3="-1.818174" y3="0.704933" z3="-0.009984" />
<atom id="a6" elementType="C" x3="-0.465924" y3="0.968973" z3="-0.040250" />
<atom id="a7" elementType="H" x3="0.749144" y3="-2.355762" z3="0.073351" />
<atom id="a8" elementType="H" x3="-1.714543" y3="-2.676719" z3="0.117433" />
<atom id="a9" elementType="O" x3="-0.021180" y3="2.236107" z3="-0.087794" />
<atom id="a10" elementType="H" x3="0.938082" y3="2.218829" z3="-0.091709" />
<atom id="a11" elementType="H" x3="-3.332992" y3="-0.801174" z3="0.076800" />
<atom id="a12" elementType="H" x3="-2.502858" y3="1.537608" z3="-0.025411" />
<atom id="a13" elementType="O" x3="1.747744" y3="0.315508" z3="-0.049161" />
<atom id="a14" elementType="C" x3="2.747637" y3="-0.671439" z3="0.053456" />
<atom id="a15" elementType="H" x3="2.726218" y3="-1.338257" z3="-0.804001" />
<atom id="a16" elementType="H" x3="3.691092" y3="-0.141544" z3="0.090132" />
<atom id="a17" elementType="H" x3="2.616966" y3="-1.259179" z3="0.959960" />

```
            <atom id="a18" elementType="O" x3="1.304094" y3="-3.417539"
z3="-0.144590" />
            <atom id="a19" elementType="H" x3="0.830776" y3="-3.720477"
z3="-0.925759" />
         </atomArray>
         <bondArray>
            <bond atomRefs2="a19 a18" order="1" />
            <bond atomRefs2="a15 a14" order="1" />
            <bond atomRefs2="a18 a7" order="1" />
            <bond atomRefs2="a10 a9" order="1" />
            <bond atomRefs2="a9 a6" order="1" />
            <bond atomRefs2="a13 a1" order="1" />
            <bond atomRefs2="a13 a14" order="1" />
            <bond atomRefs2="a6 a1" order="2" />
            <bond atomRefs2="a6 a5" order="1" />
            <bond atomRefs2="a12 a5" order="1" />
            <bond atomRefs2="a1 a2" order="1" />
            <bond atomRefs2="a5 a4" order="2" />
            <bond atomRefs2="a2 a3" order="2" />
            <bond atomRefs2="a4 a3" order="1" />
            <bond atomRefs2="a4 a11" order="1" />
            <bond atomRefs2="a14 a16" order="1" />
            <bond atomRefs2="a14 a17" order="1" />
            <bond atomRefs2="a3 a8" order="1" />
         </bondArray>
         <propertyList>
            <property title="program">
               <scalar>Gaussian 09, Revision B.01</scalar>
            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
            <property title="method">
               <scalar>umpwb95</scalar>
            </property>
            <property title="File Format">
               <scalar>g03</scalar>
            </property>
            <property title="MW">
               <scalar>141.145</scalar>
            </property>
            <property title="Energy" dictRef="me:ZPE">
               <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">5.33</scalar>
```

```
            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
              <scalar>2.00</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
              <array units="cm-1">62.46 102.25 131.11 169.46 198.99 250.22 289.85
325.35 347.11 368.78 462.87 485.93 516.97 572.97 579.49 612.89 704.22 735.88
787.42 831.96 906.57 919.98 989.74 996.92 1095.29 1129.85 1179.92 1201.19
1216.46 1238.02 1297.00 1324.06 1361.87 1416.13 1441.74 1513.25 1534.24
1539.62 1552.82 1593.56 1692.75 1726.48 3121.77 3210.65 3253.36 3278.43
3293.76 3303.29 3924.43 3930.19</array>
            </property>
            <property title="ImaginaryFrequency" dictRef="me:imFreqs">
              <scalar units="cm-1">1714.27</scalar>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
              <array units="cm-1">0.057 0.040 0.024</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
              <scalar>1</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
              <scalar>1</scalar>
            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
        <molecule id="oh" spinMultiplicity="2">
          <atomArray>
            <atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000"
y3="0.000000" z3="0.107474" />
            <atom id="a2" elementType="H" x3="0.000000" y3="0.000000"
z3="-0.859789" />
          </atomArray>
          <bondArray>
            <bond atomRefs2="a2 a1" order="1" />
          </bondArray>
          <propertyList>
            <property title="program">
              <scalar>Gaussian 09, Revision B.01</scalar>
            </property>
            <property title="basis">
              <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
```

```
            <property title="method">
               <scalar>umpwb95</scalar>
            </property>
            <property title="File Format">
               <scalar>g03</scalar>
            </property>
            <property title="MW">
               <scalar>17.0073</scalar>
            </property>
            <property title="Energy" dictRef="me:ZPE">
               <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
               <scalar>2.00</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
               <array units="cm-1">3870.53</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
               <array units="cm-1">18.991</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
               <scalar>1</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
      </molecule>
   </moleculeList>
   <reactionList>
      <reaction id="r1" reversible="true">
         <reactantList>
            <reactant>
               <molecule ref="R1b" role="deficientReactant" />
            </reactant>
            <reactant>
               <molecule ref="oh" role="excessReactant" />
            </reactant>
         </reactantList>
         <productList>
            <product>
```

```
            <molecule ref="IM9" role="modelled" />
          </product>
        </productList>
        <me:transitionState>
          <molecule ref="TS9" role="transitionState" />
        </me:transitionState>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
```

```
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_193309</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
```

Guaiacol + OH → IM10 + H_2O

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190902_162259" />
    </molecule>
    <molecule id="IM10" spinMultiplicity="2">
      <atomArray>
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z3="-0.000029" />
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</property>

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1234.18 1260.62 1300.55 1326.28 1342.21 1361.87 1447.00 1501.15 1522.42
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
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    <dc:date>20190908_193519</dc:date>
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Guaiacol + OH → IM11 + H_2O

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xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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            <bond atomRefs2="a13 a15" order="1" />
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            </property>
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               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
```

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            </property>
            <property title="File Format">
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            </property>
            <property title="MW">
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            </property>
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zeroPointVibEnergyAdded="true">-3.36</scalar>
            </property>
            <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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481.24 516.61 558.68 560.26 596.66 711.09 795.02 795.65 850.03 872.29 942.46
1093.30 1120.35 1176.36 1205.97 1232.20 1263.98 1288.86 1322.97 1369.89
1439.47 1494.14 1514.82 1529.10 1544.66 1587.31 1694.73 1723.07 3100.54
3175.92 3246.62 3284.93 3292.00 3301.32 3922.29</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
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            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
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z3="0.000077" />
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z3="0.000036" />
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z3="0.000160" />
    <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
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    <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
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z3="-0.000245" />
    <atom id="a11" elementType="H" x3="-3.335842" y3="-0.786514"
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    <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
    <atom id="a13" elementType="O" x3="1.738049" y3="0.317486"
z3="-0.000027" />
    <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
    <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
z3="-0.889139" />
    <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
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<bond atomRefs2="a13 a1" order="1" />
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</property>
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<bond atomRefs2="a12 a5" order="1" />
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803.95 827.18 895.12 911.15 957.87 1077.69 1107.01 1129.27 1184.69 1205.21
1231.16 1264.84 1299.77 1323.03 1337.24 1369.79 1438.19 1512.71 1517.45
1526.70 1543.09 1601.57 1712.71 1717.33 3102.20 3178.29 3248.74 3293.19
3300.16 3308.08 3923.61 3926.61</array>
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               <molecule ref="oh" role="excessReactant" />
            </reactant>
         </reactantList>
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        </me:transitionState>
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        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
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    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
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    </me:conditions>
    <me:modelParameters>
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
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    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
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    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
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    <dc:date>20190908_193714</dc:date>
    <dc:contributor>Administrator</dc:contributor>
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</me:mesmer>
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Guaiacol + OH → IM12 + H_2O

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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1086.60 1123.18 1187.61 1203.66 1211.47 1246.56 1312.57 1328.34 1363.74
1414.22 1510.54 1530.92 1533.14 1548.13 1593.92 1666.36 1736.79 3102.68
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         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
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z3="0.000077" />
    <atom id="a3" elementType="C" x3="-1.374750" y3="-1.635679"
z3="0.000036" />
    <atom id="a4" elementType="C" x3="-2.275327" y3="-0.589898"
z3="-0.000055" />
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z3="-0.000072" />
    <atom id="a6" elementType="C" x3="-0.471454" y3="0.983504"
z3="0.000041" />
    <atom id="a7" elementType="H" x3="0.693038" y3="-2.198155"
z3="0.000160" />
    <atom id="a8" elementType="H" x3="-1.722805" y3="-2.656359"
z3="-0.000061" />
    <atom id="a9" elementType="O" x3="-0.021706" y3="2.252155"
z3="0.000074" />
    <atom id="a10" elementType="H" x3="0.936931" y3="2.229396"
z3="-0.000245" />
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z3="-0.000161" />
    <atom id="a12" elementType="H" x3="-2.509201" y3="1.554954"
z3="-0.000129" />
    <atom id="a13" elementType="O" x3="1.738049" y3="0.317486"
z3="-0.000027" />
    <atom id="a14" elementType="C" x3="2.721698" y3="-0.679512"
z3="-0.000063" />
    <atom id="a15" elementType="H" x3="2.644448" y3="-1.304660"
z3="-0.889139" />
    <atom id="a16" elementType="H" x3="3.676916" y3="-0.169138"
z3="-0.000547" />
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z3="0.889410" />
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    <bond atomRefs2="a10 a9" order="1" />
    <bond atomRefs2="a11 a4" order="1" />
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<bond atomRefs2="a14 a17" order="1" />
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</property>
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<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
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</property>
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<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>124.137</scalar>
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</property>
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</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
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<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
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</property>
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<atom id="a4" elementType="C" x3="-2.357047" y3="-0.833950" z3="-0.003830" />
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<atom id="a6" elementType="C" x3="-0.659685" y3="0.879098" z3="-0.101304" />
<atom id="a7" elementType="H" x3="0.734460" y3="-2.199074" z3="0.107593" />
<atom id="a8" elementType="H" x3="-1.633743" y3="-2.841544" z3="0.131392" />
<atom id="a9" elementType="O" x3="-0.329476" y3="2.182736" z3="-0.184041" />
<atom id="a10" elementType="H" x3="0.627168" y3="2.253024" z3="-0.183952" />
<atom id="a11" elementType="H" x3="-3.400283" y3="-1.105399" z3="0.005711" />
<atom id="a12" elementType="H" x3="-2.827104" y3="1.417738" z3="-0.152982" />
<atom id="a13" elementType="O" x3="1.590388" y3="0.387386" z3="-0.055368" />
<atom id="a14" elementType="C" x3="2.653154" y3="-0.526120" z3="-0.000953" />
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<atom id="a16" elementType="H" x3="3.562636" y3="0.059942" z3="-0.044830" />
<atom id="a17" elementType="H" x3="2.631558" y3="-1.093719" z3="0.928398" />

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z3="-0.230009" />
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z3="-0.262073" />
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            <bond atomRefs2="a6 a5" order="2" />
            <bond atomRefs2="a6 a1" order="1" />
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            <bond atomRefs2="a1 a2" order="2" />
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            <bond atomRefs2="a14 a17" order="1" />
            <bond atomRefs2="a2 a3" order="1" />
            <bond atomRefs2="a2 a7" order="1" />
            <bond atomRefs2="a3 a8" order="1" />
         </bondArray>
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            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
            <property title="method">
               <scalar>umpwb95</scalar>
            </property>
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            </property>
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            </property>
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310.06 343.01 379.14 436.12 477.89 519.64 555.90 572.09 635.72 696.52 753.00
775.54 808.10 862.38 898.80 915.84 991.97 1116.17 1122.08 1192.31 1203.41
1215.98 1233.55 1312.73 1324.78 1354.36 1419.57 1498.49 1509.69 1523.54
1539.90 1545.89 1606.90 1692.84 1734.67 3105.14 3182.80 3248.87 3280.95
3298.17 3305.74 3899.22 3926.26</array>
            </property>
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            </property>
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            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
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          </propertyList>
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y3="0.000000" z3="0.107474" />
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z3="-0.859789" />
          </atomArray>
          <bondArray>
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          </bondArray>
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            <property title="program">
              <scalar>Gaussian 09, Revision B.01</scalar>
            </property>
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              <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
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zeroPointVibEnergyAdded="true">0</scalar>
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   </moleculeList>
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            <reactant>
               <molecule ref="oh" role="excessReactant" />
            </reactant>
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            <molecule ref="IM12" role="modelled" />
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        </productList>
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          <molecule ref="TS12" role="transitionState" />
        </me:transitionState>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
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```
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
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    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_193859</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
```

Creosol + OH → IM1

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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      <propertyList>
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          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom"
content="E:\rate11.2\Mesmer-5.0/librarymols.xml" timestamp="20190831_112222"
/>
    </molecule>
    <molecule id="IM1" spinMultiplicity="2">
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z3="0.025944" />
        <atom id="a3" elementType="C" spinMultiplicity="2" x3="1.876192"
y3="0.274964" z3="-0.020845" />
        <atom id="a4" elementType="C" x3="1.775141" y3="-1.124498"
z3="-0.151112" />
        <atom id="a5" elementType="C" x3="0.580193" y3="-1.762146"
z3="-0.195701" />
        <atom id="a6" elementType="C" x3="-0.710904" y3="-1.052772"
z3="-0.009909" />
        <atom id="a7" elementType="H" x3="0.763642" y3="2.115660"
```

```
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z3="-0.830450" />
            <atom    id="a10"    elementType="H"    x3="2.685248"    y3="-1.701421"
z3="-0.233096" />
            <atom    id="a11"    elementType="H"    x3="0.501172"    y3="-2.831034"
z3="-0.315954" />
            <atom    id="a12"    elementType="O"    x3="-1.715755"    y3="1.058182"
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z3="-0.038464" />
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z3="-0.910816" />
            <atom    id="a15"    elementType="H"    x3="-2.776515"    y3="2.751529"
z3="-0.077295" />
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z3="0.866751" />
            <atom    id="a17"    elementType="O"    x3="-1.320300"    y3="-1.439535"
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            <atom    id="a18"    elementType="H"    x3="-0.716819"    y3="-1.250698"
z3="1.930533" />
            <atom    id="a19"    elementType="C"    x3="3.197706"    y3="0.958139"
z3="0.044744" />
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z3="-0.713386" />
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z3="-0.105967" />
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<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
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</property>
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<scalar>155.171</scalar>
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<scalar>2.00</scalar>
</property>
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</property>

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            </property>
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            </property>
            <property dictRef="me:sigma" default="true">
               <scalar>5.0</scalar>
            </property>
            <property dictRef="me:epsilon" default="true">
               <scalar>50.0</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
      <molecule id="R3a" spinMultiplicity="1" default="true">
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z3="0.000065" />
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z3="-0.000049" />
            <atom id="a3" elementType="C" x3="1.716632" y3="-0.348662"
z3="-0.000152" />
            <atom id="a4" elementType="C" x3="1.799795" y3="1.031038"
z3="-0.000216" />
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</property>
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</property>
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            <molecule ref="oh" role="excessReactant" />
          </reactant>
        </reactantList>
        <productList>
          <product>
            <molecule ref="IM1" role="modelled" />
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          <A>1.000e-011</A>
          <n>0</n>
          <E>0</E>
        </rateParameters>
        <me:MCRCMethod default="true DefinedSumOfStates,
LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
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      <me:PTs>
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bathGas="He" />
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    <me:modelParameters>
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      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
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    </me:modelParameters>
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      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
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      <dc:date>20190908_201740</dc:date>
      <dc:contributor>Administrator</dc:contributor>
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</me:mesmer>
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Creosol + OH → IM2

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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  <moleculeList convention="">
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</property>
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<atom id="a12" elementType="O" x3="-1.961048" y3="-0.616382" z3="0.000105" />
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851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77
1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40
1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72
3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
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          <property title="MW">
            <scalar>17.0073</scalar>
          </property>
          <property title="Energy" dictRef="me:ZPE">
            <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
          </property>
          <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
            <scalar>2.00</scalar>
          </property>
          <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
            <array units="cm-1">3870.53</array>
          </property>
          <property title="Rotational Constants" dictRef="me:rotConsts">
            <array units="cm-1">18.991</array>
          </property>
          <property title="Symmetry Number" dictRef="me:symmetryNumber">
            <scalar>1</scalar>
          </property>
          <property dictRef="me:frequenciesScaleFactor" default="true">
            <scalar>1</scalar>
          </property>
        </propertyList>
        <me:DOSCMethod default="true" name="ClassicalRotors" />
      </molecule>
    </moleculeList>
    <reactionList>
      <reaction id="r1" reversible="true">
```

```
        <reactantList>
          <reactant>
            <molecule ref="R3a" role="deficientReactant" />
          </reactant>
          <reactant>
            <molecule ref="oh" role="excessReactant" />
          </reactant>
        </reactantList>
        <productList>
          <product>
            <molecule ref="IM2" role="modelled" />
          </product>
        </productList>
        <rateParameters reactionType="arrhenius" reversible="true">
          <A>3.000e-011</A>
          <n>0</n>
          <E>0</E>
        </rateParameters>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
        <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294" precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
```

```
  <me:control>
    <me:testDOS />
    <me:printSpeciesProfile />
    <!--<me:testMicroRates />-->
    <me:testRateConstant />
    <me:printGrainDOS />
    <!--<me:printCellDOS />-->
    <!--<me:printReactionOperatorColumnSums />-->
    <!--<me:printTunnellingCoefficients />-->
    <me:printGrainkfE />
    <!--<me:printGrainBoltzmann />-->
    <me:printGrainkbE />
    <me:eigenvalues>0</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_202207</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
```

Creosol + OH → IM3

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190902_140548" />
    </molecule>
    <molecule id="IM3" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.759854" y3="-0.015937"
z3="-0.056099" />
        <atom id="a2" elementType="C" x3="-0.491716" y3="-0.814112"
z3="-0.092307" />
        <atom id="a3" elementType="C" x3="-1.723758" y3="0.031978"
z3="-0.183539" />
        <atom id="a4" elementType="C" x3="-1.644526" y3="1.383554"
z3="-0.097112" />
        <atom id="a5" elementType="C" spinMultiplicity="2" x3="-0.418251"
y3="2.068686" z3="0.019293" />
        <atom id="a6" elementType="C" x3="0.775205" y3="1.346897"
z3="0.035813" />
        <atom id="a7" elementType="H" x3="-0.472208" y3="-1.504730"
z3="-0.941380" />
```

```
            <atom id="a8" elementType="O" x3="1.945161" y3="2.013430"
z3="0.138253" />
            <atom id="a9" elementType="H" x3="2.652299" y3="1.365717"
z3="0.135000" />
            <atom id="a10" elementType="H" x3="-2.555798" y3="1.963482"
z3="-0.129638" />
            <atom id="a11" elementType="H" x3="-0.378690" y3="3.142962"
z3="0.087986" />
            <atom id="a12" elementType="O" x3="1.966142" y3="-0.627013"
z3="0.019203" />
            <atom id="a13" elementType="C" x3="2.089350" y3="-1.923800"
z3="-0.518719" />
            <atom id="a14" elementType="H" x3="1.891793" y3="-1.916800"
z3="-1.590271" />
            <atom id="a15" elementType="H" x3="3.116411" y3="-2.223397"
z3="-0.348877" />
            <atom id="a16" elementType="H" x3="1.417645" y3="-2.615208"
z3="-0.017129" />
            <atom id="a17" elementType="O" x3="-0.553205" y3="-1.703885"
z3="1.025318" />
            <atom id="a18" elementType="H" x3="-0.559375" y3="-1.171449"
z3="1.821126" />
            <atom id="a19" elementType="C" x3="-3.006313" y3="-0.706146"
z3="-0.332481" />
            <atom id="a20" elementType="H" x3="-3.114801" y3="-1.459200"
z3="0.446348" />
            <atom id="a21" elementType="H" x3="-3.857225" y3="-0.032707"
z3="-0.288220" />
            <atom id="a22" elementType="H" x3="-3.043905" y3="-1.235650"
z3="-1.286224" />
         </atomArray>
         <bondArray>
            <bond atomRefs2="a14 a13" order="1" />
            <bond atomRefs2="a22 a19" order="1" />
            <bond atomRefs2="a7 a2" order="1" />
            <bond atomRefs2="a13 a15" order="1" />
            <bond atomRefs2="a13 a16" order="1" />
            <bond atomRefs2="a13 a12" order="1" />
            <bond atomRefs2="a19 a21" order="1" />
            <bond atomRefs2="a19 a3" order="1" />
            <bond atomRefs2="a19 a20" order="1" />
            <bond atomRefs2="a3 a4" order="2" />
            <bond atomRefs2="a3 a2" order="1" />
            <bond atomRefs2="a10 a4" order="1" />
```

<bond atomRefs2="a4 a5" order="1" />
<bond atomRefs2="a2 a1" order="1" />
<bond atomRefs2="a2 a17" order="1" />
<bond atomRefs2="a1 a12" order="1" />
<bond atomRefs2="a1 a6" order="2" />
<bond atomRefs2="a5 a6" order="1" />
<bond atomRefs2="a5 a11" order="1" />
<bond atomRefs2="a6 a8" order="1" />
<bond atomRefs2="a9 a8" order="1" />
<bond atomRefs2="a17 a18" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>155.171</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">-17.61</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">64.87 114.24 134.25 163.71 189.12 205.76 252.96 262.95 307.36 346.02 363.08 410.02 443.02 461.07 487.99 515.74 582.50 597.12 662.31 738.19 770.53 808.07 910.90 940.67 1000.96 1038.27 1067.38 1097.91 1137.13 1193.94 1204.55 1225.31 1231.42 1237.23 1297.52 1326.23 1353.64 1398.90 1422.89 1438.88 1448.78 1471.93 1501.56 1520.95 1524.83 1527.35 1547.66 1646.01 1691.23 3072.77 3097.82 3107.06 3166.65 3194.96 3214.24 3244.48 3260.12 3307.85 3937.14 3946.00</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">

```
            <array units="cm-1">0.049 0.036 0.022</array>
          </property>
          <property title="Symmetry Number" dictRef="me:symmetryNumber">
            <scalar>1</scalar>
          </property>
          <property dictRef="me:sigma" default="true">
            <scalar>5.0</scalar>
          </property>
          <property dictRef="me:epsilon" default="true">
            <scalar>50.0</scalar>
          </property>
          <property dictRef="me:frequenciesScaleFactor" default="true">
            <scalar>1</scalar>
          </property>
        </propertyList>
        <me:DOSCMethod default="true" name="ClassicalRotors" />
        <me:DistributionCalcMethod default="true" name="Boltzmann" />
        <me:energyTransferModel name="ExponentialDown" default="true" />
        <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
      <molecule id="R3a" spinMultiplicity="1" default="true">
        <atomArray>
          <atom id="a1" elementType="C" x3="-0.683939" y3="-0.157132"
z3="0.000065" />
          <atom id="a2" elementType="C" x3="0.451856" y3="-0.937909"
z3="-0.000049" />
          <atom id="a3" elementType="C" x3="1.716632" y3="-0.348662"
z3="-0.000152" />
          <atom id="a4" elementType="C" x3="1.799795" y3="1.031038"
z3="-0.000216" />
          <atom id="a5" elementType="C" x3="0.657565" y3="1.821694"
z3="-0.000085" />
          <atom id="a6" elementType="C" x3="-0.585706" y3="1.234999"
z3="0.000072" />
          <atom id="a7" elementType="H" x3="0.372378" y3="-2.013983"
z3="-0.000093" />
          <atom id="a8" elementType="O" x3="-1.703238" y3="1.988128"
z3="0.000135" />
          <atom id="a9" elementType="H" x3="-2.459326" y3="1.398704"
z3="0.000163" />
          <atom id="a10" elementType="H" x3="2.769036" y3="1.506751"
z3="-0.000386" />
          <atom id="a11" elementType="H" x3="0.721581" y3="2.898224"
z3="-0.000173" />
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<atom id="a12" elementType="O" x3="-1.961048" y3="-0.616382" z3="0.000105" />
<atom id="a13" elementType="C" x3="-2.163910" y3="-2.001778" z3="-0.000147" />
<atom id="a14" elementType="H" x3="-1.732954" y3="-2.460794" z3="0.889090" />
<atom id="a15" elementType="H" x3="-3.236182" y3="-2.154764" z3="-0.000214" />
<atom id="a16" elementType="H" x3="-1.732882" y3="-2.460474" z3="-0.889515" />
<atom id="a17" elementType="C" x3="2.943084" y3="-1.206905" z3="0.000208" />
<atom id="a18" elementType="H" x3="2.980830" y3="-1.847033" z3="0.879939" />
<atom id="a19" elementType="H" x3="2.976555" y3="-1.853961" z3="-0.874579" />
<atom id="a20" elementType="H" x3="3.842991" y3="-0.598712" z3="-0.004333" />
</atomArray>
<bondArray>
<bond atomRefs2="a16 a13" order="1" />
<bond atomRefs2="a19 a17" order="1" />
<bond atomRefs2="a20 a17" order="1" />
<bond atomRefs2="a10 a4" order="1" />
<bond atomRefs2="a4 a3" order="2" />
<bond atomRefs2="a4 a5" order="1" />
<bond atomRefs2="a15 a13" order="1" />
<bond atomRefs2="a11 a5" order="1" />
<bond atomRefs2="a3 a2" order="1" />
<bond atomRefs2="a3 a17" order="1" />
<bond atomRefs2="a13 a12" order="1" />
<bond atomRefs2="a13 a14" order="1" />
<bond atomRefs2="a7 a2" order="1" />
<bond atomRefs2="a5 a6" order="2" />
<bond atomRefs2="a2 a1" order="2" />
<bond atomRefs2="a1 a6" order="1" />
<bond atomRefs2="a1 a12" order="1" />
<bond atomRefs2="a6 a8" order="1" />
<bond atomRefs2="a8 a9" order="1" />
<bond atomRefs2="a17 a18" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>

```
            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
            <property title="method">
               <scalar>umpwb95</scalar>
            </property>
            <property title="File Format">
               <scalar>g03</scalar>
            </property>
            <property title="MW">
               <scalar>138.164</scalar>
            </property>
            <property title="Energy" dictRef="me:ZPE">
               <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
               <array units="cm-1">19.81 77.69 151.16 193.76 208.81 266.95 301.95
369.10 373.00 445.48 472.34 474.99 564.19 580.61 609.68 730.76 741.43 840.62
851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77
1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40
1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72
3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
               <array units="cm-1">0.064 0.039 0.025</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
               <scalar>1</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
      </molecule>
      <molecule id="oh" spinMultiplicity="2">
         <atomArray>
            <atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000"
y3="0.000000" z3="0.107474" />
            <atom id="a2" elementType="H" x3="0.000000" y3="0.000000"
z3="-0.859789" />
         </atomArray>
```

```
        <bondArray>
          <bond atomRefs2="a2 a1" order="1" />
        </bondArray>
        <propertyList>
          <property title="program">
            <scalar>Gaussian 09, Revision B.01</scalar>
          </property>
          <property title="basis">
            <scalar>6-31+G(d,p) (6D, 7F)</scalar>
          </property>
          <property title="method">
            <scalar>umpwb95</scalar>
          </property>
          <property title="File Format">
            <scalar>g03</scalar>
          </property>
          <property title="MW">
            <scalar>17.0073</scalar>
          </property>
          <property title="Energy" dictRef="me:ZPE">
            <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
          </property>
          <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
            <scalar>2.00</scalar>
          </property>
          <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
            <array units="cm-1">3870.53</array>
          </property>
          <property title="Rotational Constants" dictRef="me:rotConsts">
            <array units="cm-1">18.991</array>
          </property>
          <property title="Symmetry Number" dictRef="me:symmetryNumber">
            <scalar>1</scalar>
          </property>
          <property dictRef="me:frequenciesScaleFactor" default="true">
            <scalar>1</scalar>
          </property>
        </propertyList>
        <me:DOSCMethod default="true" name="ClassicalRotors" />
      </molecule>
    </moleculeList>
    <reactionList>
      <reaction id="r1" reversible="true">
```

```
        <reactantList>
          <reactant>
            <molecule ref="R3a" role="deficientReactant" />
          </reactant>
          <reactant>
            <molecule ref="oh" role="excessReactant" />
          </reactant>
        </reactantList>
        <productList>
          <product>
            <molecule ref="IM3" role="modelled" />
          </product>
        </productList>
        <rateParameters reactionType="arrhenius" reversible="true">
          <A>3.500e-011</A>
          <n>0</n>
          <E>0</E>
        </rateParameters>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
        <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
```

```
  <me:control>
    <me:testDOS />
    <me:printSpeciesProfile />
    <!--<me:testMicroRates />-->
    <me:testRateConstant />
    <me:printGrainDOS />
    <!--<me:printCellDOS />-->
    <!--<me:printReactionOperatorColumnSums />-->
    <!--<me:printTunnellingCoefficients />-->
    <me:printGrainkfE />
    <!--<me:printGrainBoltzmann />-->
    <me:printGrainkbE />
    <me:eigenvalues>0</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_230020</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
```

Creosol + OH → IM4

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190905_160824" />
    </molecule>
    <molecule id="IM4" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.902731" y3="-0.161958"
z3="-0.008935" />
        <atom id="a2" elementType="C" x3="-0.226191" y3="-0.898637"
z3="0.012041" />
        <atom id="a3" elementType="C" x3="-1.587380" y3="-0.277346"
z3="0.025585" />
        <atom id="a4" elementType="C" spinMultiplicity="2" x3="-1.528750"
y3="1.217016" z3="0.015140" />
        <atom id="a5" elementType="C" x3="-0.369066" y3="1.919735"
z3="-0.006817" />
        <atom id="a6" elementType="C" x3="0.863203" y3="1.260032"
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</property>
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</property>
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        </propertyList>
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        <me:deltaEDown default="true">250.0</me:deltaEDown>
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            </property>
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369.10 373.00 445.48 472.34 474.99 564.19 580.61 609.68 730.76 741.43 840.62
851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77
1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40
1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72
3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
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y3="0.000000" z3="0.107474" />
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          <property title="basis">
            <scalar>6-31+G(d,p) (6D, 7F)</scalar>
          </property>
          <property title="method">
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        <productList>
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          <n>0</n>
          <E>0</E>
        </rateParameters>
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        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
        <me:TInfinity default="true">298</me:TInfinity>
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      <me:bathGas>He</me:bathGas>
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      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
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    <me:printSpeciesProfile />
    <!--<me:testMicroRates />-->
    <me:testRateConstant />
    <me:printGrainDOS />
    <!--<me:printCellDOS />-->
    <!--<me:printReactionOperatorColumnSums />-->
    <!--<me:printTunnellingCoefficients />-->
    <me:printGrainkfE />
    <!--<me:printGrainBoltzmann />-->
    <me:printGrainkbE />
    <me:eigenvalues>0</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
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    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_202446</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
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Creosol + OH → IM5

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<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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  <moleculeList convention="">
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<bond atomRefs2="a6 a8" order="1" />
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            </property>
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               <array units="cm-1">19.81 77.69 151.16 193.76 208.81 266.95 301.95
369.10 373.00 445.48 472.34 474.99 564.19 580.61 609.68 730.76 741.43 840.62
851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77
1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40
1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72
3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
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y3="0.000000" z3="0.107474" />
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z3="-0.859789" />
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          </property>
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        </propertyList>
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            <molecule ref="R3a" role="deficientReactant" />
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            <molecule ref="oh" role="excessReactant" />
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        </reactantList>
        <productList>
          <product>
            <molecule ref="IM5" role="modelled" />
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          <n>0</n>
          <E>0</E>
        </rateParameters>
        <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
        <me:TInfinity default="true">298</me:TInfinity>
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    </reactionList>
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        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
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    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
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    <me:printSpeciesProfile />
    <!--<me:testMicroRates />-->
    <me:testRateConstant />
    <me:printGrainDOS />
    <!--<me:printCellDOS />-->
    <!--<me:printReactionOperatorColumnSums />-->
    <!--<me:printTunnellingCoefficients />-->
    <me:printGrainkfE />
    <!--<me:printGrainBoltzmann />-->
    <me:printGrainkbE />
    <me:eigenvalues>0</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>bve.xml</dc:source>
    <dc:creator>Mesmer v5.0</dc:creator>
    <dc:date>20190908_202726</dc:date>
    <dc:contributor>Administrator</dc:contributor>
  </metadataList>
</me:mesmer>
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Creosol + OH → IM6

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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        <property dictRef="me:sigma">
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        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
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content="E:\rate11.2\Mesmer-5.0/librarymols.xml" timestamp="20190831_105535"
/>
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z3="-0.202594" />
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z3="-0.234500" />
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z3="1.142587" />
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z3="0.026395" />
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z3="-0.782720" />
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            <bond atomRefs2="a5 a17" order="1" />
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            <bond atomRefs2="a10 a4" order="1" />
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</property>
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<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
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<scalar>2.00</scalar>
</property>
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</property>

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            </property>
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         </propertyList>
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         <me:deltaEDown default="true">250.0</me:deltaEDown>
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z3="0.000065" />
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z3="-0.000049" />
            <atom id="a3" elementType="C" x3="1.716632" y3="-0.348662"
z3="-0.000152" />
            <atom id="a4" elementType="C" x3="1.799795" y3="1.031038"
z3="-0.000216" />
            <atom id="a5" elementType="C" x3="0.657565" y3="1.821694"
z3="-0.000085" />
            <atom id="a6" elementType="C" x3="-0.585706" y3="1.234999"
z3="0.000072" />
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z3="-0.000093" />
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z3="0.000135" />
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z3="0.000105" />
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            <atom id="a19" elementType="H" x3="2.976555" y3="-1.853961"
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</property>
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<property title="MW">
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<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
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<array units="cm-1">19.81 77.69 151.16 193.76 208.81 266.95 301.95 369.10 373.00 445.48 472.34 474.99 564.19 580.61 609.68 730.76 741.43 840.62 851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77 1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40 1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72 3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
</property>
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</property>
</propertyList>
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        <!--...or by the total number of grains
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        <!--Specify increased energy range
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        <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
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        <me:printSpeciesProfile />
        <!--<me:testMicroRates />-->
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        <me:printGrainDOS />
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        <!--<me:printReactionOperatorColumnSums />-->
        <!--<me:printTunnellingCoefficients />-->
        <me:printGrainkfE />
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        <me:printGrainkbE />
        <me:eigenvalues>0</me:eigenvalues>
        <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
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        <!--Adjusts displayed energies to this values for the lowest species. -->
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      <dc:date>20190908_202848</dc:date>
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Creosol + OH → IM7 + H_2O

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881.76 966.84 1002.49 1036.21 1061.58 1105.64 1173.12 1200.92 1208.93 1241.85
1270.89 1340.24 1379.93 1439.67 1471.79 1498.48 1509.22 1509.82 1523.38
1532.11 1554.51 1575.56 1602.86 1681.85 3103.09 3113.74 3179.46 3182.04
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
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      <me:printGrainkfE />
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      <me:printGrainkbE />
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      <!--Adjusts displayed energies to this values for the lowest species. -->
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Creosol + OH → IM8 + H_2O

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          <n>0</n>
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        </rateParameters>
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        <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
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      <me:PTs>
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    </me:conditions>
    <me:modelParameters>
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
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      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_203752</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
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Creosol + OH → IM9 + H_2O

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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            <property dictRef="me:sigma">
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/>
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y3="-0.886024" z3="-0.000019" />
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</property>
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<property dictRef="me:epsilon" default="true">

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851.66 886.27 969.75 975.13 1043.30 1079.38 1123.38 1174.14 1204.73 1225.77
1254.54 1264.48 1324.93 1356.47 1372.68 1443.01 1454.37 1498.18 1515.40
1520.20 1520.26 1539.43 1547.51 1625.97 1732.44 1745.56 3100.37 3113.72
3175.17 3181.52 3210.95 3244.44 3270.41 3283.45 3296.61 3922.65</array>
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y3="0.216760" z3="-0.000030" />
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            <atom id="a6" elementType="C" x3="1.509724" y3="-0.865754"
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            <molecule ref="oh" role="excessReactant" />
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    </reactionList>
    <me:conditions>
      <me:bathGas>He</me:bathGas>
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        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
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    </me:conditions>
    <me:modelParameters>
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_204207</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
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Creosol + OH → IM10 + H_2O

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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  <moleculeList convention="">
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        <property dictRef="me:sigma">
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</property>
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</property>
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</property>
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</property>
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            <reactant>
               <molecule ref="oh" role="excessReactant" />
            </reactant>
         </reactantList>
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         </productList>
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LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
         <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
      </reaction>
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      <me:bathGas>He</me:bathGas>
      <me:PTs>
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        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_204401</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Creosol + OH → IM11 + H_2O

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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        <atom elementType="He" />
      </atomArray>
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        </property>
        <property dictRef="me:sigma">
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        </property>
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<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
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</property>
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</property>
<property title="MW">
<scalar>137.156</scalar>
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            <property dictRef="me:frequenciesScaleFactor" default="true">
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</property>
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<property dictRef="me:frequenciesScaleFactor" default="true">
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      </property>
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220.17 287.45 309.82 328.71 370.06 426.70 442.18 469.00 475.06 563.27 577.72
614.37 705.17 726.03 770.04 857.83 873.50 904.59 993.39 1049.71 1075.20 1096.02
1135.67 1205.50 1221.85 1240.78 1262.02 1298.40 1312.87 1337.52 1373.73
1448.19 1451.30 1491.59 1521.35 1524.53 1528.30 1531.33 1543.66 1609.99
1707.50 1733.33 3103.05 3117.60 3179.51 3185.83 3227.90 3247.55 3284.78
3298.15 3920.80 3929.24</array>
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            </property>
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            </reactant>
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         </productList>
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LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
         <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
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      <me:PTs>
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    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_211008</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Creosol + OH → IM12 + H_2O

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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        <atom elementType="He" />
      </atomArray>
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          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
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        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
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timestamp="20190907_155608" />
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z3="-0.001420" />
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      </property>
      <property title="method">
        <scalar>umpwb95</scalar>
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      <property title="File Format">
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        <scalar>137.156</scalar>
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zeroPointVibEnergyAdded="true">-2.07</scalar>
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      <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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347.05 371.75 437.65 466.16 491.87 562.02 586.78 590.60 708.96 719.61 843.38
847.46 884.77 977.49 1043.92 1074.91 1099.15 1200.62 1202.94 1232.90 1259.28
1305.90 1330.30 1377.01 1419.66 1444.04 1490.10 1515.98 1517.74 1518.51
1533.32 1539.42 1612.51 1663.44 1747.73 3102.53 3116.29 3178.58 3186.12
3214.18 3246.44 3271.99 3292.66 3924.49</array>
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      <property title="Symmetry Number" dictRef="me:symmetryNumber">
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            <atom id="a15" elementType="H" x3="-3.236182" y3="-2.154764"
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</property>
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<property dictRef="me:frequenciesScaleFactor" default="true">
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250.65 292.58 306.29 351.31 362.06 402.73 428.91 472.13 477.77 568.96 585.38
598.04 690.72 762.72 783.45 828.23 872.32 904.99 907.00 988.23 1044.65 1077.42
1122.42 1205.71 1210.80 1247.25 1256.27 1313.75 1320.74 1370.36 1429.12
1446.12 1495.68 1503.95 1516.51 1520.20 1533.37 1539.12 1551.56 1621.50
1701.83 1744.73 3103.89 3116.57 3181.65 3186.19 3215.75 3247.82 3280.76
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            </property>
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zeroPointVibEnergyAdded="true">0</scalar>
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         <productList>
            <product>
               <molecule ref="IM12" role="modelled" />
            </product>
         </productList>
         <me:transitionState>
            <molecule ref="TS12" role="transitionState" />
         </me:transitionState>
         <me:MCRCMethod default="true DefinedSumOfStates,
LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT,
SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="SimpleRRKM" />
         <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
      </reaction>
   </reactionList>
   <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
```

```
        <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
        <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
        <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
        <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_211555</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
```

Syringol + OH → IM1

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190903_093103" />
    </molecule>
    <molecule id="IM1" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="-1.229282" y3="0.169538"
z3="-0.010064" />
        <atom id="a2" elementType="C" x3="-1.203137" y3="1.526386"
z3="0.030297" />
        <atom id="a3" elementType="C" spinMultiplicity="2" x3="0.030418"
y3="2.200608" z3="0.059919" />
        <atom id="a4" elementType="C" x3="1.241632" y3="1.492718"
z3="0.011434" />
        <atom id="a5" elementType="C" x3="1.253115" y3="0.131382"
z3="-0.037400" />
        <atom id="a6" elementType="C" x3="0.002039" y3="-0.690661"
z3="0.066549" />
        <atom id="a7" elementType="H" x3="-2.117736" y3="2.096721"
z3="0.017189" />
```

<atom id="a8" elementType="H" x3="0.046071" y3="3.277173" z3="0.097832" />
<atom id="a9" elementType="O" x3="0.008337" y3="-1.638630" z3="-0.936161" />
<atom id="a10" elementType="H" x3="-0.787656" y3="-2.161461" z3="-0.825501" />
<atom id="a11" elementType="H" x3="2.168010" y3="2.043101" z3="-0.000230" />
<atom id="a12" elementType="O" x3="-2.322008" y3="-0.604559" z3="-0.094102" />
<atom id="a13" elementType="C" x3="-3.569643" y3="0.026559" z3="-0.176134" />
<atom id="a14" elementType="H" x3="-3.626208" y3="0.662465" z3="-1.059014" />
<atom id="a15" elementType="H" x3="-4.308594" y3="-0.761849" z3="-0.247205" />
<atom id="a16" elementType="H" x3="-3.760948" y3="0.625275" z3="0.714043" />
<atom id="a17" elementType="O" x3="-0.009855" y3="-1.416713" z3="1.281972" />
<atom id="a18" elementType="H" x3="-0.127477" y3="-0.805174" z3="2.008024" />
<atom id="a19" elementType="O" x3="2.335592" y3="-0.641070" z3="-0.106199" />
<atom id="a20" elementType="C" x3="3.585885" y3="-0.016304" z3="-0.165436" />
<atom id="a21" elementType="H" x3="3.768064" y3="0.581103" z3="0.728202" />
<atom id="a22" elementType="H" x3="4.319531" y3="-0.810475" z3="-0.225300" />
<atom id="a23" elementType="H" x3="3.664262" y3="0.619549" z3="-1.047112" />
</atomArray>
<bondArray>
<bond atomRefs2="a14 a13" order="1" />
<bond atomRefs2="a23 a20" order="1" />
<bond atomRefs2="a9 a10" order="1" />
<bond atomRefs2="a9 a6" order="1" />
<bond atomRefs2="a15 a13" order="1" />
<bond atomRefs2="a22 a20" order="1" />
<bond atomRefs2="a13 a12" order="1" />
<bond atomRefs2="a13 a16" order="1" />
<bond atomRefs2="a20 a19" order="1" />
<bond atomRefs2="a20 a21" order="1" />

<bond atomRefs2="a19 a5" order="1" />
<bond atomRefs2="a12 a1" order="1" />
<bond atomRefs2="a5 a4" order="2" />
<bond atomRefs2="a5 a6" order="1" />
<bond atomRefs2="a1 a2" order="2" />
<bond atomRefs2="a1 a6" order="1" />
<bond atomRefs2="a11 a4" order="1" />
<bond atomRefs2="a4 a3" order="1" />
<bond atomRefs2="a7 a2" order="1" />
<bond atomRefs2="a2 a3" order="1" />
<bond atomRefs2="a3 a8" order="1" />
<bond atomRefs2="a6 a17" order="1" />
<bond atomRefs2="a17 a18" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>171.171</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">-22.75</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">43.92 89.55 108.42 189.92 202.56 224.31 248.03 268.84 290.14 298.38 308.95 330.75 358.77 360.74 412.09 482.57 503.98 591.65 631.29 664.03 702.84 725.74 748.93 831.27 879.98 904.07 952.41 1073.51 1097.93 1130.90 1141.52 1173.79 1178.24 1203.24 1204.04 1238.29 1242.78 1304.35 1328.32 1354.09 1390.82 1417.09 1461.60 1497.05 1514.34 1526.55 1530.67 1539.97 1543.38 1546.68 1613.27 1690.06 3094.93 3099.93 3168.12 3175.07 3246.60

```
3246.77 3285.66 3294.16 3307.79 3943.87 3969.48</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
               <array units="cm-1">0.059 0.024 0.019</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
               <scalar>1</scalar>
            </property>
            <property dictRef="me:sigma" default="true">
               <scalar>5.0</scalar>
            </property>
            <property dictRef="me:epsilon" default="true">
               <scalar>50.0</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
      <molecule id="R2a" spinMultiplicity="1" default="true">
         <atomArray>
            <atom id="a1" elementType="C" x3="1.185702" y3="0.040390"
z3="-0.000074" />
            <atom id="a2" elementType="C" x3="1.179043" y3="1.425105"
z3="-0.000027" />
            <atom id="a3" elementType="C" x3="-0.038733" y3="2.081089"
z3="-0.000070" />
            <atom id="a4" elementType="C" x3="-1.229717" y3="1.376450"
z3="-0.000112" />
            <atom id="a5" elementType="C" x3="-1.215231" y3="-0.012435"
z3="-0.000045" />
            <atom id="a6" elementType="C" x3="0.001594" y3="-0.684004"
z3="-0.000131" />
            <atom id="a7" elementType="H" x3="2.099736" y3="1.983838"
z3="0.000163" />
            <atom id="a8" elementType="H" x3="-0.061178" y3="3.159248"
z3="-0.000138" />
            <atom id="a9" elementType="O" x3="0.020154" y3="-2.028476"
z3="-0.000177" />
            <atom id="a10" elementType="H" x3="0.937890" y3="-2.305835"
```

```
z3="-0.000200" />
            <atom    id="a11"    elementType="H"    x3="-2.164792"    y3="1.910287"
z3="-0.000295" />
            <atom    id="a12"    elementType="O"    x3="-2.310237"    y3="-0.793340"
z3="0.000203" />
            <atom    id="a13"    elementType="C"    x3="-3.558685"    y3="-0.164712"
z3="0.000144" />
            <atom    id="a14"    elementType="H"    x3="-4.296057"    y3="-0.958254"
z3="0.000492" />
            <atom    id="a15"    elementType="H"    x3="-3.694002"    y3="0.452219"
z3="0.888954" />
            <atom    id="a16"    elementType="H"    x3="-3.694212"    y3="0.451603"
z3="-0.889062" />
            <atom    id="a17"    elementType="O"    x3="2.294608"    y3="-0.742531"
z3="-0.000088" />
            <atom    id="a18"    elementType="C"    x3="3.544153"    y3="-0.110417"
z3="0.000246" />
            <atom    id="a19"    elementType="H"    x3="4.286454"    y3="-0.899209"
z3="0.000255" />
            <atom    id="a20"    elementType="H"    x3="3.670766"    y3="0.506187"
z3="-0.888910" />
            <atom    id="a21"    elementType="H"    x3="3.670442"    y3="0.505897"
z3="0.889645" />
        </atomArray>
        <bondArray>
            <bond atomRefs2="a16 a13" order="1" />
            <bond atomRefs2="a20 a18" order="1" />
            <bond atomRefs2="a11 a4" order="1" />
            <bond atomRefs2="a10 a9" order="1" />
            <bond atomRefs2="a9 a6" order="1" />
            <bond atomRefs2="a8 a3" order="1" />
            <bond atomRefs2="a6 a1" order="2" />
            <bond atomRefs2="a6 a5" order="1" />
            <bond atomRefs2="a4 a3" order="1" />
            <bond atomRefs2="a4 a5" order="2" />
            <bond atomRefs2="a17 a1" order="1" />
            <bond atomRefs2="a17 a18" order="1" />
            <bond atomRefs2="a1 a2" order="1" />
            <bond atomRefs2="a3 a2" order="2" />
            <bond atomRefs2="a5 a12" order="1" />
            <bond atomRefs2="a2 a7" order="1" />
            <bond atomRefs2="a13 a12" order="1" />
            <bond atomRefs2="a13 a14" order="1" />
            <bond atomRefs2="a13 a15" order="1" />
```

<bond atomRefs2="a18 a19" order="1" />
<bond atomRefs2="a18 a21" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>154.163</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">61.77 93.08 166.60 213.95 231.99 276.31 305.48 335.73 346.54 373.78 385.17 453.74 512.71 547.52 574.00 613.17 639.09 740.25 741.95 784.46 860.72 880.80 964.56 976.51 1145.91 1151.64 1200.79 1206.13 1207.60 1227.90 1248.11 1251.65 1312.64 1339.30 1350.00 1396.77 1455.92 1514.08 1519.99 1536.51 1540.84 1549.28 1551.74 1572.82 1619.36 1711.11 1744.05 3091.40 3100.99 3162.60 3176.57 3240.48 3243.36 3283.87 3307.25 3314.76 3936.07</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.077 0.026 0.020</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>

```
<molecule id="oh" spinMultiplicity="2">
  <atomArray>
    <atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.000000" z3="0.107474" />
    <atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
  </atomArray>
  <bondArray>
    <bond atomRefs2="a2 a1" order="1" />
  </bondArray>
  <propertyList>
    <property title="program">
      <scalar>Gaussian 09, Revision B.01</scalar>
    </property>
    <property title="basis">
      <scalar>6-31+G(d,p) (6D, 7F)</scalar>
    </property>
    <property title="method">
      <scalar>umpwb95</scalar>
    </property>
    <property title="File Format">
      <scalar>g03</scalar>
    </property>
    <property title="MW">
      <scalar>17.0073</scalar>
    </property>
    <property title="Energy" dictRef="me:ZPE">
      <scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
    </property>
    <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
      <scalar>2.00</scalar>
    </property>
    <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
      <array units="cm-1">3870.53</array>
    </property>
    <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">18.991</array>
    </property>
    <property title="Symmetry Number" dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor" default="true">
      <scalar>1</scalar>
```

```
            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
      </moleculeList>
      <reactionList>
        <reaction id="r1" reversible="true">
          <reactantList>
            <reactant>
              <molecule ref="R2a" role="deficientReactant" />
            </reactant>
            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM1" role="modelled" />
            </product>
          </productList>
          <rateParameters reactionType="arrhenius" reversible="true">
            <A>2.500e-011</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
          <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
          <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
          <me:TInfinity default="true">298</me:TInfinity>
        </reaction>
      </reactionList>
      <me:conditions>
        <me:bathGas>He</me:bathGas>
        <me:PTs>
          <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
          <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
          <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
          <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
        </me:PTs>
      </me:conditions>
      <me:modelParameters>
        <!--Specify grain size directly...-->
```

```
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
   <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_194458</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
```

Syringol + OH → IM2

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema" xmlns:me="http://www.chem.leeds.ac.uk/mesmer" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml" timestamp="20190903_094528" />
    </molecule>
    <molecule id="IM2" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="-1.132100" y3="0.052625" z3="0.200205" />
        <atom id="a2" elementType="C" x3="-1.001454" y3="1.522309" z3="0.031277" />
        <atom id="a3" elementType="C" x3="0.207597" y3="2.108799" z3="-0.062998" />
        <atom id="a4" elementType="C" spinMultiplicity="2" x3="1.422383" y3="1.372384" z3="-0.078272" />
        <atom id="a5" elementType="C" x3="1.390404" y3="-0.012060" z3="-0.029932" />
        <atom id="a6" elementType="C" x3="0.172543" y3="-0.661985" z3="0.044403" />
        <atom id="a7" elementType="H" x3="-1.909209" y3="2.104011" z3="0.061228" />
```

<atom id="a8" elementType="H" x3="0.268370" y3="3.184656" z3="-0.132586" />
<atom id="a9" elementType="O" x3="0.116099" y3="-1.988238" z3="0.044812" />
<atom id="a10" elementType="H" x3="-0.810161" y3="-2.237837" z3="-0.026427" />
<atom id="a11" elementType="H" x3="2.357142" y3="1.900431" z3="-0.148034" />
<atom id="a12" elementType="O" x3="-1.982075" y3="-0.585276" z3="-0.709245" />
<atom id="a13" elementType="C" x3="-3.320218" y3="-0.150861" z3="-0.725620" />
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      <!--Specify increased energy range
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are not shown-->
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Syringol + OH → IM3

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SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
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      <!--...or by the total number of grains
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
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      <!--<me:testMicroRates />-->
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      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
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Syringol + OH → IM4

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741.95 784.46 860.72 880.80 964.56 976.51 1145.91 1151.64 1200.79 1206.13
1207.60 1227.90 1248.11 1251.65 1312.64 1339.30 1350.00 1396.77 1455.92
1514.08 1519.99 1536.51 1540.84 1549.28 1551.74 1572.82 1619.36 1711.11
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3314.76 3936.07</array>
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<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
</atomArray>
<bondArray>
<bond atomRefs2="a2 a1" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
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</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>17.0073</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">3870.53</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">18.991</array>
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<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>

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            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
      </moleculeList>
      <reactionList>
        <reaction id="r1" reversible="true">
          <reactantList>
            <reactant>
              <molecule ref="R2a" role="deficientReactant" />
            </reactant>
            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM4" role="modelled" />
            </product>
          </productList>
          <rateParameters reactionType="arrhenius" reversible="true">
            <A>5.000e-012</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
          <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
          <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
          <me:TInfinity default="true">298</me:TInfinity>
        </reaction>
      </reactionList>
      <me:conditions>
        <me:bathGas>He</me:bathGas>
        <me:PTs>
          <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
          <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
          <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
          <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
        </me:PTs>
      </me:conditions>
      <me:modelParameters>
        <!--Specify grain size directly...-->
```

```
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
   <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_195134</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
```

Syringol + OH → IM5

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190903_095642" />
    </molecule>
    <molecule id="IM5" spinMultiplicity="2">
      <atomArray>
        <atom id="a1" elementType="C" x3="-1.391588" y3="0.006646"
z3="-0.040558" />
        <atom id="a2" elementType="C" x3="-1.237951" y3="1.380029"
z3="-0.254683" />
        <atom id="a3" elementType="C" spinMultiplicity="2" x3="0.006564"
y3="1.918588" z3="-0.368014" />
        <atom id="a4" elementType="C" x3="1.251125" y3="1.122202"
z3="-0.207402" />
        <atom id="a5" elementType="C" x3="0.989529" y3="-0.338315"
z3="-0.055790" />
        <atom id="a6" elementType="C" x3="-0.267708" y3="-0.843553"
z3="0.057945" />
        <atom id="a7" elementType="H" x3="-2.104982" y3="2.015297"
z3="-0.339842" />
```

```
            <atom id="a8" elementType="H" x3="0.134747" y3="2.976816"
z3="-0.531066" />
            <atom id="a9" elementType="O" x3="-0.455213" y3="-2.164584"
z3="0.253438" />
            <atom id="a10" elementType="H" x3="-1.399180" y3="-2.325465"
z3="0.284592" />
            <atom id="a11" elementType="H" x3="1.906055" y3="1.291755"
z3="-1.065767" />
            <atom id="a12" elementType="O" x3="-2.571474" y3="-0.640387"
z3="0.083852" />
            <atom id="a13" elementType="C" x3="-3.754522" y3="0.102268"
z3="-0.037838" />
            <atom id="a14" elementType="H" x3="-3.816003" y3="0.579776"
z3="-1.014738" />
            <atom id="a15" elementType="H" x3="-4.569781" y3="-0.601969"
z3="0.071771" />
            <atom id="a16" elementType="H" x3="-3.822189" y3="0.858842"
z3="0.742635" />
            <atom id="a17" elementType="O" x3="2.043385" y3="1.608664"
z3="0.878714" />
            <atom id="a18" elementType="H" x3="1.529277" y3="1.514701"
z3="1.680710" />
            <atom id="a19" elementType="O" x3="2.019196" y3="-1.189606"
z3="0.082787" />
            <atom id="a20" elementType="C" x3="3.256105" y3="-0.834628"
z3="-0.483873" />
            <atom id="a21" elementType="H" x3="3.647570" y3="0.078939"
z3="-0.043291" />
            <atom id="a22" elementType="H" x3="3.926384" y3="-1.658257"
z3="-0.268876" />
            <atom id="a23" elementType="H" x3="3.171618" y3="-0.722561"
z3="-1.565188" />
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            <bond atomRefs2="a11 a4" order="1" />
            <bond atomRefs2="a14 a13" order="1" />
            <bond atomRefs2="a8 a3" order="1" />
            <bond atomRefs2="a20 a22" order="1" />
            <bond atomRefs2="a20 a21" order="1" />
            <bond atomRefs2="a20 a19" order="1" />
            <bond atomRefs2="a3 a2" order="1" />
            <bond atomRefs2="a3 a4" order="1" />
            <bond atomRefs2="a7 a2" order="1" />
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<bond atomRefs2="a2 a1" order="2" />
<bond atomRefs2="a4 a5" order="1" />
<bond atomRefs2="a4 a17" order="1" />
<bond atomRefs2="a5 a6" order="2" />
<bond atomRefs2="a5 a19" order="1" />
<bond atomRefs2="a1 a6" order="1" />
<bond atomRefs2="a1 a12" order="1" />
<bond atomRefs2="a13 a15" order="1" />
<bond atomRefs2="a13 a12" order="1" />
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<bond atomRefs2="a6 a9" order="1" />
<bond atomRefs2="a9 a10" order="1" />
<bond atomRefs2="a17 a18" order="1" />
</bondArray>
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</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>171.171</scalar>
</property>
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<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">-16.20</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">59.18 80.98 122.63 153.01 200.73 213.14 229.92 242.35 263.73 305.31 335.37 347.12 384.11 394.48 415.02 468.90 491.33 556.52 564.32 634.43 691.62 698.96 733.34 832.73 935.47 941.26 1012.61 1082.85 1133.32 1179.90 1201.41 1202.45 1216.69 1234.26 1238.93 1239.57 1279.81 1330.26 1346.30 1382.02 1415.61 1429.32 1471.66 1505.88 1519.59 1525.79 1530.38 1541.42 1547.66 1560.32 1632.82 1719.55 3087.59 3103.91 3104.83 3181.70

```
3196.78 3243.38 3248.21 3284.20 3301.29 3941.41 3952.86</array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
               <array units="cm-1">0.056 0.023 0.017</array>
            </property>
            <property title="Symmetry Number" dictRef="me:symmetryNumber">
               <scalar>1</scalar>
            </property>
            <property dictRef="me:sigma" default="true">
               <scalar>5.0</scalar>
            </property>
            <property dictRef="me:epsilon" default="true">
               <scalar>50.0</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
      </molecule>
      <molecule id="R2a" spinMultiplicity="1" default="true">
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z3="-0.000074" />
            <atom id="a2" elementType="C" x3="1.179043" y3="1.425105"
z3="-0.000027" />
            <atom id="a3" elementType="C" x3="-0.038733" y3="2.081089"
z3="-0.000070" />
            <atom id="a4" elementType="C" x3="-1.229717" y3="1.376450"
z3="-0.000112" />
            <atom id="a5" elementType="C" x3="-1.215231" y3="-0.012435"
z3="-0.000045" />
            <atom id="a6" elementType="C" x3="0.001594" y3="-0.684004"
z3="-0.000131" />
            <atom id="a7" elementType="H" x3="2.099736" y3="1.983838"
z3="0.000163" />
            <atom id="a8" elementType="H" x3="-0.061178" y3="3.159248"
z3="-0.000138" />
            <atom id="a9" elementType="O" x3="0.020154" y3="-2.028476"
z3="-0.000177" />
            <atom id="a10" elementType="H" x3="0.937890" y3="-2.305835"
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z3="-0.000200" />
            <atom    id="a11"    elementType="H"    x3="-2.164792"    y3="1.910287"
z3="-0.000295" />
            <atom    id="a12"    elementType="O"    x3="-2.310237"    y3="-0.793340"
z3="0.000203" />
            <atom    id="a13"    elementType="C"    x3="-3.558685"    y3="-0.164712"
z3="0.000144" />
            <atom    id="a14"    elementType="H"    x3="-4.296057"    y3="-0.958254"
z3="0.000492" />
            <atom    id="a15"    elementType="H"    x3="-3.694002"    y3="0.452219"
z3="0.888954" />
            <atom    id="a16"    elementType="H"    x3="-3.694212"    y3="0.451603"
z3="-0.889062" />
            <atom    id="a17"    elementType="O"    x3="2.294608"    y3="-0.742531"
z3="-0.000088" />
            <atom    id="a18"    elementType="C"    x3="3.544153"    y3="-0.110417"
z3="0.000246" />
            <atom    id="a19"    elementType="H"    x3="4.286454"    y3="-0.899209"
z3="0.000255" />
            <atom    id="a20"    elementType="H"    x3="3.670766"    y3="0.506187"
z3="-0.888910" />
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z3="0.889645" />
        </atomArray>
        <bondArray>
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            <bond atomRefs2="a20 a18" order="1" />
            <bond atomRefs2="a11 a4" order="1" />
            <bond atomRefs2="a10 a9" order="1" />
            <bond atomRefs2="a9 a6" order="1" />
            <bond atomRefs2="a8 a3" order="1" />
            <bond atomRefs2="a6 a1" order="2" />
            <bond atomRefs2="a6 a5" order="1" />
            <bond atomRefs2="a4 a3" order="1" />
            <bond atomRefs2="a4 a5" order="2" />
            <bond atomRefs2="a17 a1" order="1" />
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            <bond atomRefs2="a1 a2" order="1" />
            <bond atomRefs2="a3 a2" order="2" />
            <bond atomRefs2="a5 a12" order="1" />
            <bond atomRefs2="a2 a7" order="1" />
            <bond atomRefs2="a13 a12" order="1" />
            <bond atomRefs2="a13 a14" order="1" />
            <bond atomRefs2="a13 a15" order="1" />
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<bond atomRefs2="a18 a19" order="1" />
<bond atomRefs2="a18 a21" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>154.163</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">61.77 93.08 166.60 213.95 231.99 276.31 305.48 335.73 346.54 373.78 385.17 453.74 512.71 547.52 574.00 613.17 639.09 740.25 741.95 784.46 860.72 880.80 964.56 976.51 1145.91 1151.64 1200.79 1206.13 1207.60 1227.90 1248.11 1251.65 1312.64 1339.30 1350.00 1396.77 1455.92 1514.08 1519.99 1536.51 1540.84 1549.28 1551.74 1572.82 1619.36 1711.11 1744.05 3091.40 3100.99 3162.60 3176.57 3240.48 3243.36 3283.87 3307.25 3314.76 3936.07</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.077 0.026 0.020</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>

<molecule id="oh" spinMultiplicity="2">
<atomArray>
<atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.000000" z3="0.107474" />
<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
</atomArray>
<bondArray>
<bond atomRefs2="a2 a1" order="1" />
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision B.01</scalar>
</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>17.0073</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">3870.53</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">18.991</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>

```
            </property>
          </propertyList>
          <me:DOSCMethod default="true" name="ClassicalRotors" />
        </molecule>
      </moleculeList>
      <reactionList>
        <reaction id="r1" reversible="true">
          <reactantList>
            <reactant>
              <molecule ref="R2a" role="deficientReactant" />
            </reactant>
            <reactant>
              <molecule ref="oh" role="excessReactant" />
            </reactant>
          </reactantList>
          <productList>
            <product>
              <molecule ref="IM5" role="modelled" />
            </product>
          </productList>
          <rateParameters reactionType="arrhenius" reversible="true">
            <A>1.500e-011</A>
            <n>0</n>
            <E>0</E>
          </rateParameters>
          <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
          <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
          <me:TInfinity default="true">298</me:TInfinity>
        </reaction>
      </reactionList>
      <me:conditions>
        <me:bathGas>He</me:bathGas>
        <me:PTs>
          <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
          <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
          <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
          <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
        </me:PTs>
      </me:conditions>
      <me:modelParameters>
        <!--Specify grain size directly...-->
```

```
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
   <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_195354</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
```

Syringol + OH → IM6

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
      <atomArray>
        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
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1138.98 1192.44 1201.64 1207.40 1219.96 1237.17 1248.12 1313.36 1342.34
1347.98 1373.83 1469.24 1489.73 1515.05 1531.82 1536.39 1542.95 1547.25
1552.07 1580.12 1681.23 1701.31 3105.05 3108.49 3182.39 3197.59 3245.06
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      <!--Specify increased energy range
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      <dc:contributor>Administrator</dc:contributor>
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</me:mesmer>
```

Syringol + OH → IM7 + H_2O

```
<?xml version="1.0" encoding="utf-8" ?>
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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
    <molecule id="He">
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        <atom elementType="He" />
      </atomArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>10.2</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="F:\Mesmer-5.0/librarymols.xml"
timestamp="20190903_153836" />
    </molecule>
    <molecule id="IM7" spinMultiplicity="2">
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z3="-0.000022" />
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z3="0.000046" />
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y3="2.020728" z3="0.000100" />
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z3="0.000090" />
        <atom id="a5" elementType="C" x3="1.235404" y3="-0.025026"
z3="0.000022" />
        <atom id="a6" elementType="C" x3="0.000053" y3="-0.792065"
z3="-0.000034" />
        <atom id="a7" elementType="H" x3="-2.135616" y3="1.919195"
z3="0.000058" />
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<atom id="a11" elementType="O" x3="2.327516" y3="-0.776827" z3="0.000004" />
<atom id="a12" elementType="C" x3="3.575183" y3="-0.138196" z3="0.000055" />
<atom id="a13" elementType="H" x3="4.316118" y3="-0.927445" z3="0.000029" />
<atom id="a14" elementType="H" x3="3.699985" y3="0.477995" z3="-0.889670" />
<atom id="a15" elementType="H" x3="3.699957" y3="0.477908" z3="0.889845" />
<atom id="a16" elementType="O" x3="-2.327457" y3="-0.777086" z3="-0.000076" />
<atom id="a17" elementType="C" x3="-3.575002" y3="-0.138253" z3="-0.000088" />
<atom id="a18" elementType="H" x3="-4.316078" y3="-0.927369" z3="-0.000145" />
<atom id="a19" elementType="H" x3="-3.699683" y3="0.477901" z3="0.889683" />
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<bond atomRefs2="a4 a3" order="1" />
<bond atomRefs2="a4 a10" order="1" />
<bond atomRefs2="a3 a8" order="1" />
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</property>
<property title="basis">
<scalar>6-31+G(d,p) (6D, 7F)</scalar>
</property>
<property title="method">
<scalar>umpwb95</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="MW">
<scalar>153.155</scalar>
</property>
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<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">-33.50</scalar>
</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
<scalar>2.00</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
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</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:sigma" default="true">
<scalar>5.0</scalar>

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            </property>
            <property dictRef="me:epsilon" default="true">
               <scalar>50.0</scalar>
            </property>
            <property dictRef="me:frequenciesScaleFactor" default="true">
               <scalar>1</scalar>
            </property>
         </propertyList>
         <me:DOSCMethod default="true" name="ClassicalRotors" />
         <me:DistributionCalcMethod default="true" name="Boltzmann" />
         <me:energyTransferModel name="ExponentialDown" default="true" />
         <me:deltaEDown default="true">250.0</me:deltaEDown>
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z3="-0.000074" />
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z3="-0.000027" />
            <atom id="a3" elementType="C" x3="-0.038733" y3="2.081089"
z3="-0.000070" />
            <atom id="a4" elementType="C" x3="-1.229717" y3="1.376450"
z3="-0.000112" />
            <atom id="a5" elementType="C" x3="-1.215231" y3="-0.012435"
z3="-0.000045" />
            <atom id="a6" elementType="C" x3="0.001594" y3="-0.684004"
z3="-0.000131" />
            <atom id="a7" elementType="H" x3="2.099736" y3="1.983838"
z3="0.000163" />
            <atom id="a8" elementType="H" x3="-0.061178" y3="3.159248"
z3="-0.000138" />
            <atom id="a9" elementType="O" x3="0.020154" y3="-2.028476"
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            <atom id="a10" elementType="H" x3="0.937890" y3="-2.305835"
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            <atom id="a11" elementType="H" x3="-2.164792" y3="1.910287"
z3="-0.000295" />
            <atom id="a12" elementType="O" x3="-2.310237" y3="-0.793340"
z3="0.000203" />
            <atom id="a13" elementType="C" x3="-3.558685" y3="-0.164712"
z3="0.000144" />
            <atom id="a14" elementType="H" x3="-4.296057" y3="-0.958254"
z3="0.000492" />
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z3="0.888954" />
            <atom    id="a16"    elementType="H"    x3="-3.694212"    y3="0.451603"
z3="-0.889062" />
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z3="-0.000088" />
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z3="0.000246" />
            <atom    id="a19"    elementType="H"    x3="4.286454"    y3="-0.899209"
z3="0.000255" />
            <atom    id="a20"    elementType="H"    x3="3.670766"    y3="0.506187"
z3="-0.888910" />
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z3="0.889645" />
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            <bond atomRefs2="a1 a2" order="1" />
            <bond atomRefs2="a3 a2" order="2" />
            <bond atomRefs2="a5 a12" order="1" />
            <bond atomRefs2="a2 a7" order="1" />
            <bond atomRefs2="a13 a12" order="1" />
            <bond atomRefs2="a13 a14" order="1" />
            <bond atomRefs2="a13 a15" order="1" />
            <bond atomRefs2="a18 a19" order="1" />
            <bond atomRefs2="a18 a21" order="1" />
         </bondArray>
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            </property>
            <property title="basis">
               <scalar>6-31+G(d,p) (6D, 7F)</scalar>
            </property>
```

<property title="method">
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</property>
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<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
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<array units="cm-1">61.77 93.08 166.60 213.95 231.99 276.31 305.48 335.73 346.54 373.78 385.17 453.74 512.71 547.52 574.00 613.17 639.09 740.25 741.95 784.46 860.72 880.80 964.56 976.51 1145.91 1151.64 1200.79 1206.13 1207.60 1227.90 1248.11 1251.65 1312.64 1339.30 1350.00 1396.77 1455.92 1514.08 1519.99 1536.51 1540.84 1549.28 1551.74 1572.82 1619.36 1711.11 1744.05 3091.40 3100.99 3162.60 3176.57 3240.48 3243.36 3283.87 3307.25 3314.76 3936.07</array>
</property>
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</molecule>
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</atomArray>
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</bondArray>

```
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          </property>
          <property title="basis">
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          </property>
          <property title="method">
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        </propertyList>
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    </moleculeList>
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            <reactant>
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            </reactant>
         </reactantList>
         <productList>
            <product>
               <molecule ref="IM7" role="modelled" />
            </product>
         </productList>
         <rateParameters reactionType="arrhenius" reversible="true">
            <A>3.000e-012</A>
            <n>0</n>
            <E>0</E>
         </rateParameters>
         <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
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         <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
   </reactionList>
   <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
         <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
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   </me:conditions>
   <me:modelParameters>
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
```

```
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
   </me:control>
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      <dc:title>Project name</dc:title>
      <dc:source>bve.xml</dc:source>
      <dc:creator>Mesmer v5.0</dc:creator>
      <dc:date>20190908_200023</dc:date>
      <dc:contributor>Administrator</dc:contributor>
   </metadataList>
</me:mesmer>
```

Syringol + OH → IM8 + H_2O

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<?xml version="1.0" encoding="utf-8" ?>
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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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  <moleculeList convention="">
    <molecule id="He">
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        </property>
        <property dictRef="me:sigma">
          <scalar>2.55</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">4.0</scalar>
        </property>
      </propertyList>
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<atom id="a10" elementType="H" x3="1.014438" y3="-2.292487" z3="-0.090946" />
<atom id="a11" elementType="H" x3="-2.138664" y3="1.886303" z3="0.044542" />
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<atom id="a14" elementType="H" x3="-4.226073" y3="-1.009865" z3="0.121490" />
<atom id="a15" elementType="H" x3="-3.610270" y3="0.404915" z3="0.993690" />
<atom id="a16" elementType="H" x3="-3.678571" y3="0.412727" z3="-0.783288" />
<atom id="a17" elementType="O" x3="2.367060" y3="-0.676504" z3="-0.167471" />
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<atom id="a19" elementType="H" x3="4.364412" y3="-0.818952" z3="0.132627" />
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</property>
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      <!--Specify increased energy range
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      <me:printSpeciesProfile />
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      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
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      <!--Adjusts displayed energies to this values for the lowest species. -->
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Syringol + OH → IM9 + H_2O

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      <!--...or by the total number of grains
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
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      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
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      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
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      <dc:date>20190908_200309</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
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Syringol + OH → IM10 + H_2O

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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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      <me:grainSize units="cm-1">150</me:grainSize>
      <!--...or by the total number of grains
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      <!--Specify increased energy range
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      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    </me:modelParameters>
    <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
      <!--<me:testMicroRates />-->
      <me:testRateConstant />
      <me:printGrainDOS />
      <!--<me:printCellDOS />-->
      <!--<me:printReactionOperatorColumnSums />-->
      <!--<me:printTunnellingCoefficients />-->
      <me:printGrainkfE />
      <!--<me:printGrainBoltzmann />-->
      <me:printGrainkbE />
      <me:eigenvalues>0</me:eigenvalues>
      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
      <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
      <!--Adjusts displayed energies to this values for the lowest species. -->
      <me:calcMethod default="true" name="simpleCalc" />
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      <dc:date>20190908_200525</dc:date>
      <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
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Syringol + OH → IM11 + H_2O

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xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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      <!--Specify increased energy range
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      <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
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      <dc:date>20190908_200713</dc:date>
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Syringol + OH → IM12 + H_2O

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<scalar units="kcal/mol" convention="computational" zeroPointVibEnergyAdded="true">0</scalar>
</property>
<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">61.77 93.08 166.60 213.95 231.99 276.31 305.48 335.73 346.54 373.78 385.17 453.74 512.71 547.52 574.00 613.17 639.09 740.25 741.95 784.46 860.72 880.80 964.56 976.51 1145.91 1151.64 1200.79 1206.13 1207.60 1227.90 1248.11 1251.65 1312.64 1339.30 1350.00 1396.77 1455.92 1514.08 1519.99 1536.51 1540.84 1549.28 1551.74 1572.82 1619.36 1711.11 1744.05 3091.40 3100.99 3162.60 3176.57 3240.48 3243.36 3283.87 3307.25 3314.76 3936.07</array>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.077 0.026 0.020</array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor" default="true">
<scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMethod default="true" name="ClassicalRotors" />
</molecule>
<molecule id="oh" spinMultiplicity="2">
<atomArray>
<atom id="a1" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.000000" z3="0.107474" />
<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.859789" />
</atomArray>
<bondArray>
<bond atomRefs2="a2 a1" order="1" />
</bondArray>

```
        <propertyList>
          <property title="program">
            <scalar>Gaussian 09, Revision B.01</scalar>
          </property>
          <property title="basis">
            <scalar>6-31+G(d,p) (6D, 7F)</scalar>
          </property>
          <property title="method">
            <scalar>umpwb95</scalar>
          </property>
          <property title="File Format">
            <scalar>g03</scalar>
          </property>
          <property title="MW">
            <scalar>17.0073</scalar>
          </property>
          <property title="Energy" dictRef="me:ZPE">
            <scalar units="kcal/mol" convention="computational"
zeroPointVibEnergyAdded="true">0</scalar>
          </property>
          <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
            <scalar>2.00</scalar>
          </property>
          <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
            <array units="cm-1">3870.53</array>
          </property>
          <property title="Rotational Constants" dictRef="me:rotConsts">
            <array units="cm-1">18.991</array>
          </property>
          <property title="Symmetry Number" dictRef="me:symmetryNumber">
            <scalar>1</scalar>
          </property>
          <property dictRef="me:frequenciesScaleFactor" default="true">
            <scalar>1</scalar>
          </property>
        </propertyList>
        <me:DOSCMethod default="true" name="ClassicalRotors" />
      </molecule>
    </moleculeList>
    <reactionList>
      <reaction id="r1" reversible="true">
        <reactantList>
          <reactant>
            <molecule ref="R2a" role="deficientReactant" />
```

```
            </reactant>
            <reactant>
               <molecule ref="oh" role="excessReactant" />
            </reactant>
         </reactantList>
         <productList>
            <product>
               <molecule ref="IM12" role="modelled" />
            </product>
         </productList>
         <rateParameters reactionType="arrhenius" reversible="true">
            <A>5.000e-012</A>
            <n>0</n>
            <E>0</E>
         </rateParameters>
         <me:MCRCMethod default="true DefinedSumOfStates, LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, SimpleRRKM, WKBCrossing, ZhuNakamuraCrossing" name="MesmerILT" />
         <me:excessReactantConc default="true">1e+6</me:excessReactantConc>
         <me:TInfinity default="true">298</me:TInfinity>
      </reaction>
   </reactionList>
   <me:conditions>
      <me:bathGas>He</me:bathGas>
      <me:PTs>
         <me:PTpair units="Torr" P="760" T="294." precision="d" default="true" bathGas="He" />
         <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
         <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
         <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
      </me:PTs>
   </me:conditions>
   <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">100</me:grainSize>
      <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
   </me:modelParameters>
   <me:control>
      <me:testDOS />
      <me:printSpeciesProfile />
```

```
        <!--<me:testMicroRates />-->
        <me:testRateConstant />
        <me:printGrainDOS />
        <!--<me:printCellDOS />-->
        <!--<me:printReactionOperatorColumnSums />-->
        <!--<me:printTunnellingCoefficients />-->
        <me:printGrainkfE />
        <!--<me:printGrainBoltzmann />-->
        <me:printGrainkbE />
        <me:eigenvalues>0</me:eigenvalues>
        <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false"
are not shown-->
        <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
        <!--Adjusts displayed energies to this values for the lowest species. -->
        <me:calcMethod default="true" name="simpleCalc" />
    </me:control>
    <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
        <dc:title>Project name</dc:title>
        <dc:source>bve.xml</dc:source>
        <dc:creator>Mesmer v5.0</dc:creator>
        <dc:date>20190908_201302</dc:date>
        <dc:contributor>Administrator</dc:contributor>
    </metadataList>
</me:mesmer>
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