Species dictionary

species list from RMG-java generated mechanism for bio-oil gasification

Index #	Species Name	SMILES	Molecule
1	Hyad(1)	O=CCO	
2	Aa(2)	CC(=O)O	
3	Hypp(3)	CC(=O)CO	
4	Lvgs(4)	OC1C2COC(O2)C(O)C1O	
5	Ppa(5)	CCC(=O)O	
6	Hf2o(6)	O=C1C=CCO1	
7	Isegl(7)	CC=Cc1ccc(O)c(OC)c1	
8	Phl(8)	Oc1ccccc1	
9	Sygl(9)	COc1cccc(OC)c1O	
10	H2O(10)	O	
11	CH2OOH(78)	[CH2]OO	
12	CO2(14)	O=C=O	
13	O(25)	[O]	
14	Hj(20)	[H]	
15	O2(27)	[O][O]	
16	CH3Oj(16)	C[O]	
17	H2O2(29)	OO	
18	CH2(S)(32)	[CH2]	
19	OH(26)	[OH]	
20	CH3OOH(34)	COO	
21	HCjO(22)	[CH]=O	
22	HOCO(30)	O=[C]O	
23	SPC(45)	CC[O]	
24	HO2(28)	[O]O	
25	CH2O(24)	C=O	
26	CH4(18)	C	
27	CH3OH(17)	CO	
28	CH3j(19)	[CH3]	
29	CH2(31)	[CH2]	
30	H2(21)	[H][H]	
31	C2H6(36)	CC	
32	C2H5(37)	C[CH2]	
33	CH2OH(33)	[CH2]O	
34	CH3OO(35)	CO[O]	
35	CO(15)	[C]=O	
36	CH2CO(56)	C=C=O	
37	SPC(128)	[CH2]C1OC([O])C(O)C(O)C1O	
38	CH2CHO(55)	[CH2]C=O	
39	SPC(947)	[CH2]C(OC=O)C(O)C(O)[CH]O	
40	CH3CO(54)	C[C]=O	
41	SPC(1354)	O=COC1CC(O)C(O)C1O	
42	cC2H3O(52)	[CH]1CO1	
43	SPC(50)	C=CO	
44	SPC(67)	C=[C]C	
45	CH3CHO(48)	CC=O	
46	SPC(47)	[CH2]CO	
47	C2H4(38)	C=C	
48	C2O(58)	[C]=C=O	
49	SPC(46)	C[CH]O	
50	C2(43)	[C]#[C]	
51	C2H3(39)	[CH]=C	
52	SPC(95)	CC([O])=CO	
53	C2H2(40)	C#C	
54	SPC(69)	C=C=C	
55	SPC(2282)	CC(=O)C(O)O[CH]CO	
56	SPC(2411)	[CH2]C(=O)OC(C)=CO	
57	SPC(2595)	[CH2]C(O)=CO	

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58	SPC(2596)	CC(O)=C[O]	
59	SPC(3630)	C=C(O)C(O)O[CH]CO	
60	SPC(96)	[CH2]C(=O)CO	
61	SPC(3984)	[CH2]C(=O)OC=C(C)O	
62	H3CCCH(70)	C#CC	
63	SPC(2410)	CC(=CO)OC[C]=O	
64	C3H2(72)	[CH]=C=[CH]	
65	SPC(3983)	CC(O)=COC[C]=O	
66	SPC(598)	C[C](CO)OCO	
67	SPC(2286)	C[C](CO)OC(O)C(C)=O	
68	SPC(4066)	C[C](CO)OC(C)(O)C=O	
69	SPC(4914)	[CH2]C(=O)OC(=C)CO	
70	SPC(1039)	[CH2]C(=O)OC=C	
71	SPC(3634)	C=C(O)C(O)O[C](C)CO	
72	H2CC(41)	[C]=C	
73	SPC(4913)	C=C(CO)OC[C]=O	
74	OCHCHO(59)	O=CC=O	
75	SPC(6480)	[CH2]OC(C)=CO	
76	SPC(1516)	O=COC1CC=C(O)C1O	
77	SPC(11999)	COC(C)=C[O]	
78	SPC(202)	CC=Cc1ccc(O)c([O])c1	
79	SPC(2599)	C[C]=CO	
80	SPC(1386)	CC(=O)C=O	
81	SPC(68)	[CH]=CC	
82	SPC(13966)	CC=Cc1[c]c(O)c(O)cc1	
83	SPC(14189)	CC=C[O]	
84	H2CCCH(71)	[CH]=C=C	
85	SPC(13967)	CC=[C]c1ccc(O)c(O)c1	
86	SPC(14190)	[CH2]C=CO	
87	SPC(15635)	CC(C=O)O[CH]CO	
88	SPC(16742)	C#Cc1ccc(O)c(O)c1	
89	SPC(15447)	[CH2]C(=O)OC=CC	
90	SPC(15639)	C[C](CO)OC(C)C=O	
91	SPC(66)	[CH2]C=C	
92	SPC(12257)	OC1=CCCC1O	
93	C2H(42)	[C]#C	
94	SPC(15446)	CC=COC[C]=O	
95	SPC(21200)	OC1=CCC=C1	
96	C3H6(65)	C=CC	
97	SPC(75)	C=CC=O	
98	C2H5CO(74)	CC[C]=O	
99	SPC(16081)	CC([C]=O)C=O	
100	SPC(17093)	C=CC(O)O[C](C)CO	
101	SPC(22239)	OC1=CC=C[CH]1	
102	SPC(22240)	O=C1[CH]CC=C1	
103	HCCO(57)	[CH]=C=O	
104	SPC(577)	CCO[C](C)CO	
105	HCCOH(53)	C#CO	
106	SPC(29102)	[CH]=CC(=O)C=C	
107	SPC(27511)	O=C1C=C[CH]C1	
108	SPC(29134)	[CH2]C(=O)C=C=O	
109	SPC(31475)	O=[C]COC1=CC=CC1	
110	SPC(33970)	[CH2]C(=O)OC(=C)C=C=O	
111	SPC(33391)	C1=C2C[CH]C1O2	
112	SPC(29088)	O=C1[C]=CCC1	
113	SPC(33392)	[CH]1C=C2CC1O2	
114	SPC(33390)	O=[C]C1C=CC(=O)C1	
115	SPC(15793)	CC([O])=COC(C)C=O	
116	SPC(33969)	C=C(C=C=O)OC[C]=O	
117	SPC(33396)	C=CC=C[C]=O	
118	SPC(27514)	OC1=C[C]=CC1	
119	SPC(32088)	CC(=C[O])OC1C=CCC1=O	

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120	SPC(15792)	CC(=C[O])OC(C)C=O	
121	SPC(2626)	[CH]=CC=C	
122	SPC(55084)	[CH2]CC=CC=C	
123	SPC(201)	[CH2]C=Cc1ccc(O)c(OC)c1	
124	SPC(1948)	[CH2]CC	
125	SPC(2273)	C=CC=C	
126	SPC(29714)	[C]1=CO1	
127	SPC(6556)	C#C[CH]C	
128	SPC(58432)	C=CC(O[CH]CO)c1ccc(O)c(OC)c1	
129	SPC(58436)	C=CC(O[C](C)CO)c1ccc(O)c(OC)c1	
130	SPC(59403)	C=CC([C]=O)c1ccc(O)c(OC)c1	
131	SPC(58782)	C=C=Cc1ccc(O)c(OC)c1	
132	SPC(21366)	C#CC[CH2]	
133	SPC(57964)	COc1cc(C=CCO[C](C)CO)ccc1O	
134	SPC(65830)	[CH2]C([C]=O)=Cc1ccc(O)c(OC)c1	
135	SPC(57948)	[CH]1C=CCCC1	
136	SPC(66167)	C=C=Cc1ccc(O)c([O])c1	
137	SPC(71554)	[CH]1C2CCCC12	
138	SPC(72362)	C=C=Cc1[c]c(O)c(O)cc1	
139	SPC(57947)	[CH2]C1C=CCC1	
140	SPC(58181)	COc1cc(C=CCOC(C)=C[O])ccc1O	
141	SPC(58008)	[CH2]C(=O)CC=Cc1ccc(O)c(OC)c1	
142	SPC(72364)	C#C[CH]c1ccc(O)c(O)c1	
143	SPC(75149)	[CH]1C2CC1CC2	
144	SPC(58182)	COc1cc(C=CCOC=C(C)[O])ccc1O	
145	SPC(58465)	[CH2]C(=O)C(C=C)c1ccc(O)c(OC)c1	
146	SPC(81460)	C#CC([C]=O)c1ccc(O)c(O)c1	
147	SPC(58591)	C=CC(OC(C)=C[O])c1ccc(O)c(OC)c1	
148	SPC(81295)	Oc1ccc(C=C=CC=C=Cc2ccc(O)c(O)c2)cc1O	
149	SPC(71555)	C=C=Cc1ccc(O)c(O)c1	
150	SPC(58592)	C=CC(OC=C(C)[O])c1ccc(O)c(OC)c1	
151	SPC(21482)	C#CC=C	
152	SPC(146)	O=C1C=C[CH]O1	
153	SPC(59402)	COc1cc(C=CC[C]=O)ccc1O	
154	SPC(99730)	O=[C]C=CC=O	
155	SPC(101296)	C[C](CO)OC(=O)C=CC=O	
156	SPC(101292)	O=CC=CC(=O)O[CH]CO	
157	SPC(24105)	O=CC=CC=O	
158	SPC(101364)	[CH2]C(=O)C(=O)C=CC=O	
159	SPC(2275)	[CH]=CC=O	
160	SPC(71553)	O=[C]C1C=CCCC1	
161	SPC(101363)	O=[C]CC(=O)C=CC=O	
162	SPC(91632)	[CH2]C([C]=O)=Cc1ccc(O)c(O)c1	
163	SPC(2257)	[CH2]CC=C	
164	SPC(116688)	[CH2]C(=O)C=CC=O	
165	SPC(80180)	C#CCc1ccc(O)c(O)c1	
166	SPC(2653)	[CH2]C(=C)[C]=O	
167	SPC(128881)	[CH2]C(=O)OC(=C)C=CC=O	
168	SPC(127452)	O=CC=CC(=O)CO[CH]CO	
169	SPC(15393)	C[C]=Cc1ccc(O)c(O)c1	
170	SPC(91185)	O=[C]C([CH]C=C=Cc1ccc(O)c(O)c1)=Cc1ccc(O)c(O)c1	
171	SPC(59749)	C=C[CH]C	
172	SPC(128880)	C=C(C=CC=O)OC[C]=O	
173	SPC(127456)	C[C](CO)OCC(=O)C=CC=O	
174	SPC(16743)	CC#Cc1ccc(O)c(O)c1	
175	SPC(151033)	C=CC(C)[C]=O	
176	SPC(72363)	[CH2]C#Cc1ccc(O)c(O)c1	
177	SPC(18328)	Oc1c[c]ccc1O	
178	SPC(131703)	[O]C1C=CC(=O)C1	
179	SPC(103201)	CC(=O)C=CC=O	
180	SPC(161981)	[CH2]Cc1ccc(O)c(O)c1	
181	SPC(161969)	[CH2]C(=O)c1ccc(O)c(O)c1	

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182	SPC(57996)	[CH2]OCC=Cc1ccc(O)c(OC)c1	
183	SPC(4753)	C[C](CO)OCC(=O)CO	
184	SPC(161965)	[O]C(=O)c1ccc(O)c(O)c1	
185	SPC(58457)	[CH2]OC(C=C)c1ccc(O)c(OC)c1	
186	SPC(169888)	[CH2]C(=O)OC(=C)c1ccc(O)c(O)c1	
187	SPC(162548)	Oc1[c]cccc1O	
188	SPC(168707)	C[CH]c1ccc(O)c(O)c1	
189	SPC(70978)	CC(=C[O])OC1C=CCCC1	
190	SPC(58251)	[CH2]C=COCC=Cc1ccc(O)c(OC)c1	
191	SPC(184052)	[O]c1ccccc1O	
192	SPC(183425)	[CH2]Cc1cccc(O)c1O	
193	SPC(70979)	CC([O])=COC1C=CCCC1	
194	SPC(58645)	[CH2]C=COC(C=C)c1ccc(O)c(OC)c1	
195	SPC(161946)	Oc1ccccc1O	
196	SPC(255)	COc1cccc([O])c1O	
197	SPC(183845)	COc1cccc(O)c1O	
198	SPC(203368)	COc1cc[c]c(O)c1O	
199	SPC(14635)	CC=CC[C]=O	
200	SPC(1400)	CC(=O)[C]=O	
201	SPC(160243)	[CH2]CC(=C=C)c1ccc(O)c(O)c1	
202	SPC(16626)	[C]1=CC1	
203	SPC(16566)	C=C=CC	
204	SPC(70793)	[CH2]OC1C=CCCC1	
205	SPC(2600)	CC(=O)C(O)[C]=O	
206	SPC(71550)	[CH]1CC=CCC1	
207	SPC(212401)	[CH2]C([C]=O)=CC	
208	SPC(33389)	O=[C]C1C=CCC1=O	
209	SPC(27609)	[CH2]C(=O)OC1=CCC=C1	
210	SPC(59795)	[CH2]C=CCC=C	
211	SPC(71551)	[C]1=CCCCC1	
212	SPC(31476)	[CH2]C(=O)OC1=CC=CC1	
213	SPC(237932)	C=CCC([C]=O)C=C	
214	SPC(29096)	O=[C]C1CC=CC1=O	
215	SPC(220183)	O=[C]C1CC=CCC1	
216	SPC(32185)	C[C](CO)OC1C=CC(=O)C1	
217	SPC(131695)	CC(=O)C=C[C]=O	
218	SPC(27608)	O=[C]COC1=CCC=C1	
219	SPC(2618)	[CH]=CC(C)=O	
220	SPC(259062)	CC(=O)C=CC(=O)O[C](C)CO	
221	SPC(71280)	C1=CCCC=C1	
222	SPC(70761)	C[C](CO)OC1C=CCCC1	
223	SPC(56039)	[CH2]C=CC=C[CH2]	
224	SPC(95143)	C#C[C]=C	
225	SPC(6518)	[CH]=C=CC=[CH]	
226	SPC(16620)	C=C=CC=C=C	
227	SPC(285877)	C=CC1C=CC1	
228	SPC(288452)	C=C1[C]=C1	
229	SPC(55485)	C=CC=CC=C	
230	SPC(291668)	[CH2]C([C]=O)=CC=C=C	
231	SPC(285968)	C#CC(=C)C[CH2]	
232	SPC(287954)	C#CC#C	
233	SPC(275270)	[CH]1C=CCC=C1	
234	SPC(32142)	[CH2]C=COC1C=CCC1=O	
235	SPC(160261)	[CH]=CC(=C=C)c1ccc(O)c(O)c1	
236	SPC(61968)	C#CC(C)[C]=O	
237	SPC(21370)	[CH]=CC#C	
238	SPC(312276)	[CH]=C=C=CC	
239	SPC(317333)	C1=CC2CC2[CH]1	
240	SPC(313702)	[CH2]C=COC1C=CC=CC1	
241	SPC(18193)	[CH]=Cc1ccc(O)c(O)c1	
242	SPC(315549)	C1=CCC(C2C=CC=CC2)C=C1	
243	SPC(317331)	O=[C]C1C=CC=CC1	

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244	SPC(314842)	[CH2]C=COC1C=CCC=C1	
245	SPC(161943)	C=C=C([C]=O)c1ccc(O)c(O)c1	
246	SPC(275272)	[C]1=CC=CCC1	
247	SPC(183429)	[CH]=Cc1cccc(O)c1O	
248	SPC(10609)	[CH]=C[C]=C	
249	SPC(315550)	C1=CCC(C2C=CCC=C2)C=C1	
250	SPC(313396)	[CH2]C(=O)C1C=CC=CC1	
251	CHCHOH(51)	[CH]=CO	
252	SPC(285985)	[CH]=CC(=C)C#C	
253	SPC(315804)	C1=CC(C2C=CCC=C2)C=CC1	
254	SPC(314725)	[CH2]C(=O)C1C=CCC=C1	
255	SPC(315294)	c1ccccc1	
256	SPC(317332)	O=[C]C1C=CCC=C1	
257	SPC(183409)	[O]C(=O)c1cccc(O)c1O	
258	SPC(32395)	[CH2]C=COC1C=CC(=O)C1	
259	OjCHO(23)	[O]C=O	
260	SPC(26661)	[CH2]C=COC1C=CC(O)=C1	
261	SPC(18192)	C=[C]c1ccc(O)c(O)c1	
262	SPC(26823)	[CH2]C=COC1C=CC=C1O	
263	SPC(251)	Oc1[c]cccc1	
264	SPC(18186)	C#Cc1ccc(O)c([O])c1	
265	Mofml(12)	CO[C]=O	
266	SPC(26967)	[CH2]C=COC1(O)C=CC=C1	
267	SPC(18183)	C#Cc1[c]c(O)c(O)cc1	
268	SPC(148733)	C=CC(C)O[C](C)CO	
269	SPC(32207)	[CH2]OC1C=CC(=O)C1	
270	SPC(18187)	C#Cc1ccc([O])c(O)c1	
271	SPC(254)	[O]c1ccccc1	
272	SPC(149020)	[CH2]C=COC(C)C=C	
273	SPC(18182)	[C]#Cc1ccc(O)c(O)c1	
274	SPC(18185)	C#Cc1c[c]c(O)c(O)c1	
275	SPC(149711)	[CH2]C=COCC=CC	
276	SPC(18184)	C#Cc1[c]cc(O)c(O)c1	
277	SPC(252)	Oc1c[c]ccc1	
278	SPC(13382)	CC=Cc1ccc(O)c(O)c1	
279	SPC(434665)	Oc1ccc2c(c1O)C=[C]2	
280	SPC(253)	Oc1cc[c]cc1	
281	SPC(148764)	[CH2]OC(C)C=C	
282	SPC(27522)	O=[C]C1C=CC=C1O	
283	SPC(463486)	Oc1cc2c(cc1O)C=[C]2	
284	SPC(422307)	[CH]=Cc1ccccc1O	
285	SPC(149523)	[CH2]OCC=CC	
286	SPC(27521)	O=[C]C1C=CC(O)=C1	
287	SPC(434664)	[CH]=C1c2ccc(O)c(O)c21	
288	SPC(463524)	[CH]=Cc1cccc(O)c1	
289	SPC(2244)	C=CC[C]=O	
290	SPC(26290)	OC1=CC=CC1	
291	SPC(490472)	C#Cc1[c]ccc(O)c1O	
292	SPC(422287)	[O]C(=O)c1ccccc1O	
293	SPC(26978)	O=C1C=CC=C1	
294	SPC(31962)	[CH2]C(=O)C1C=CCC1=O	
295	SPC(501221)	C#Cc1c[c]cc(O)c1O	
296	SPC(463504)	[O]C(=O)c1cccc(O)c1	
297	SPC(504103)	COc1cc(C=CCOC2=CC=C[CH]2)ccc1O	
298	SPC(517054)	C#Cc1cc[c]c(O)c1O	
299	SPC(468428)	[O]C(=O)c1ccc(O)cc1	
300	SPC(504107)	C=CC(OC1=CC=C[CH]1)c1ccc(O)c(OC)c1	
301	SPC(161944)	O=[C]CC#Cc1ccc(O)c(O)c1	
302	SPC(529513)	C#Cc1cccc([O])c1O	
303	SPC(504671)	C1=CC=C(OC2C=CC=CC2)[CH]1	
304	SPC(87498)	COc1cc(C2[CH]CCC2=O)ccc1O	
305	SPC(161740)	C=C=C(C(=C=C)c1ccc(O)c(O)c1)c1ccc(O)c(O)c1	

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306	SPC(285907)	C#CC(=C)C([O])=O	
307	SPC(162383)	C=Cc1ccc(O)c(O)c1	
308	SPC(501222)	C#Cc1cccc(O)c1[O]	
309	SPC(27530)	O=C1C=CCC1	
310	SPC(468042)	Oc1ccc2c(c1O)C#C2	
311	SPC(16624)	C#CC[C]=O	
312	SPC(501220)	[C]#Cc1cccc(O)c1O	
313	SPC(204)	COc1c[c]ccc1O	
314	SPC(16625)	C=C=C[C]=O	
315	SPC(566867)	Oc1cccc2[c]coc21	
316	SPC(575896)	COc1cc(C([O])CO)ccc1O	
317	SPC(575914)	[CH2]C(=O)c1ccc(O)c(OC)c1	
318	SPC(422288)	[CH2]Oc1ccccc1O	
319	SPC(576682)	COc1cc(C=O)ccc1O	
320	SPC(160421)	C=C=C(C=[C]c1ccc(O)c(O)c1)c1ccc(O)c(O)c1	
321	SPC(5978)	C[C]=CC	
322	SPC(287019)	[CH2]CC=C=C=C	
323	SPC(468408)	Oc1ccc2c(c1O)[C]=C2	
324	SPC(361009)	C#Cc1cccc(O)c1O	
325	SPC(588100)	[CH2]C(=O)OC(=C)c1ccc(O)c(OC)c1	
326	SPC(160422)	[CH]=C(C(=C=C)c1ccc(O)c(O)c1)c1ccc(O)c(O)c1	
327	SPC(46760)	C=C[C]=C[C]=O	
328	SPC(566866)	[CH]=C1Oc2c1cccc2O	
329	SPC(468448)	[CH]=Cc1ccc(O)cc1	
330	SPC(423264)	O=[C]c1ccccc1O	
331	SPC(588099)	C=C(OC[C]=O)c1ccc(O)c(OC)c1	
332	SPC(291619)	C#CC1C=C1	
333	SPC(6557)	C#C[CH]CC	
334	SPC(59760)	[CH2]C=CCC	
335	SPC(463485)	[CH]=C1c2cc(O)c(O)cc21	
336	SPC(464532)	O=[C]c1cccc(O)c1	
337	SPC(586554)	COc1cc(C(=O)CO[C](C)CO)ccc1O	
338	SPC(479037)	Oc1cc2c(cc1O)C#C2	
339	SPC(287037)	[CH]=CC=C=C=C	
340	SPC(95168)	C=C[C]=CC	
341	SPC(464596)	CC[CH]c1ccc(O)c(O)c1	
342	C6H5J(250)	[c]1ccccc1	
343	SPC(469454)	O=[C]c1ccc(O)cc1	
344	SPC(575913)	COc1cc(C[C]=O)ccc1O	
345	SPC(576696)	COc1cc(C(C)=O)ccc1O	
346	SPC(586550)	COc1cc(C(=O)CO[CH]CO)ccc1O	
347	SPC(184053)	[O]c1cccc(O)c1O	
348	SPC(6514)	C#C[CH]C[CH2]	
349	SPC(2241)	C=CC([O])=O	
350	SPC(655283)	[CH]=Cc1ccccc1	
351	SPC(655263)	[O]C(=O)c1ccccc1	
352	SPC(660506)	[CH2]c1ccc(O)c(OC)c1	
353	SPC(681188)	COc1cc(CO[CH]CO)ccc1O	
354	SPC(666627)	Oc1[c]ccc(O)c1O	
355	SPC(682399)	COc1cc(CCc2ccc(O)c(OC)c2)ccc1O	
356	SPC(681929)	COc1cc(COC2=CC=C[CH]2)ccc1O	
357	SPC(681192)	COc1cc(CO[C](C)CO)ccc1O	
358	SPC(666628)	[O]c1c(O)cccc1O	
359	SPC(665369)	Oc1cccc(O)c1O	
360	SPC(681204)	[CH2]OCc1ccc(O)c(OC)c1	
361	SPC(681285)	COc1cc(COC(C)=C[O])ccc1O	
362	SPC(681207)	[CH2]C(=O)Cc1ccc(O)c(OC)c1	
363	SPC(576686)	COc1cc(C)ccc1O	