Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Hydrodeoxygenation of guaiacol over orthorhombic molybdenum carbide: a DFT and microkinetic study

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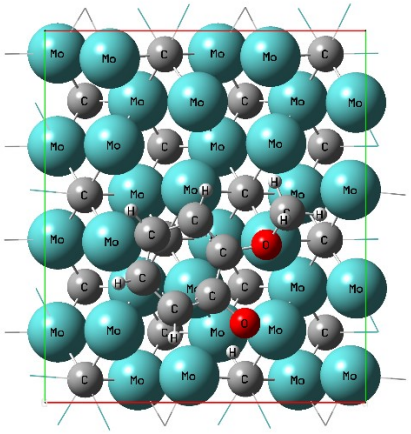
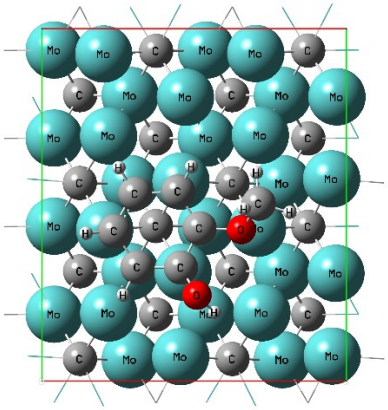
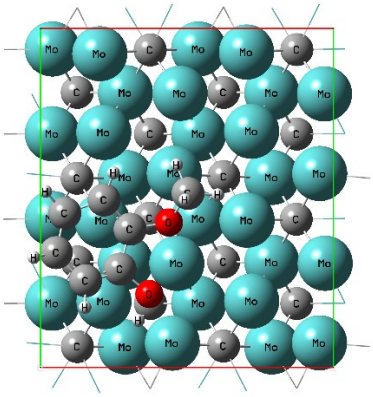
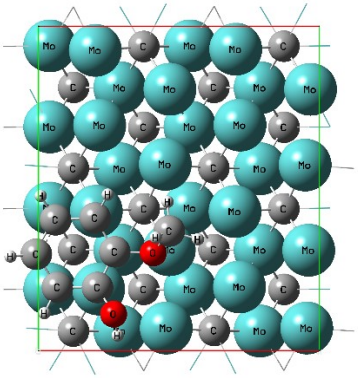
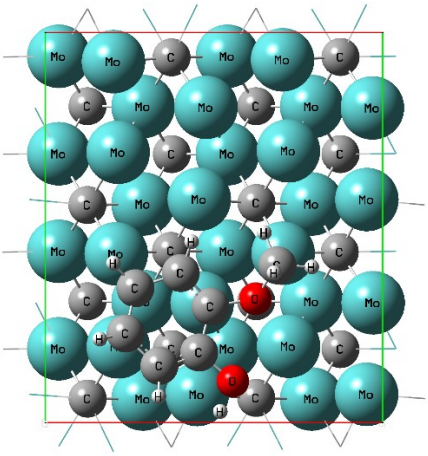
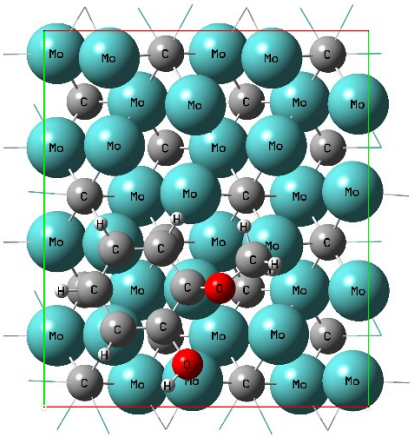
Temperature Programmed Desorption Simulation Method

In the temperature programmed desorption (TPD) simulation of the study, the microkinetic modelling of the system was conducted without considering the adsorption reactions of any species in the system. Four different cases with initial guaiacol coverage on the surface was considered (10%, 40%, 70% and 100%). For each case, at 500 K, the respective initial guaiacol coverage was considered and the ODEs of all the species were solved for time duration of 1s. The obtained concentration of all the species on the surface at the end of 1s was then considered as the initial concentration for solving the ODEs at 510K. The concentration at the end of 510 K simulation was then fed to 520 K simulation. This procedure was repeated till 700 K. This way, the concentration profile was obtained for each case of guaiacol coverage with increasing temperature. The difference between the concentration of species in the gas phase at each temperature step was calculated and plotted as a function of increasing temperature.

Table S1: Initial and final geometries of the adsorption of guaiacol via the *methoxy* group facing the surface at *atop*, *bridge*, C-*hcp*, Mo-*hcp* and *fcc* positions along with their respective adsorption energies (E_{ads}); the atoms are represented as: grey (Carbon), white (hydrogen), red (oxygen) and teal (molybdenum)

Position	Initial geometry	Final geometry	E_{ads} (eV)
atop			-4.67
bridge			-4.49
C-*hcp*			-4.67

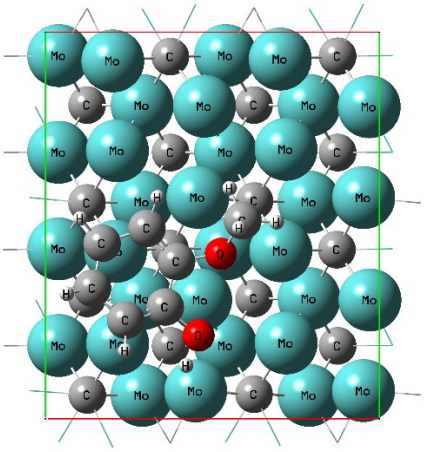
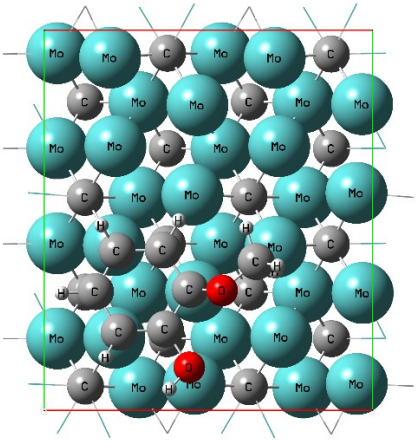
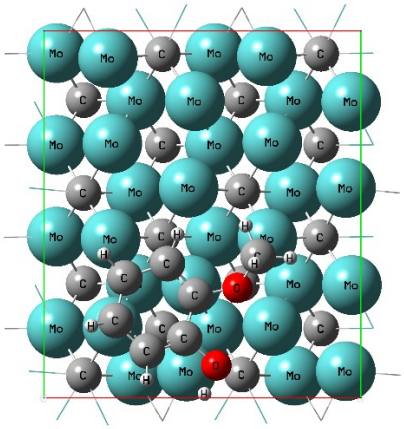
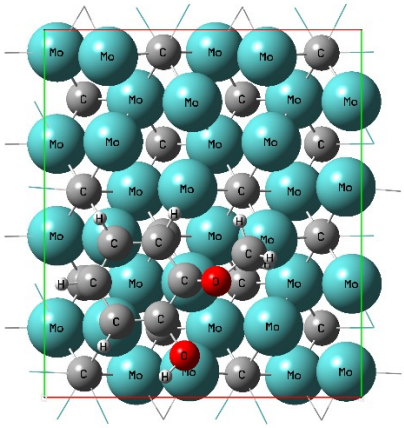
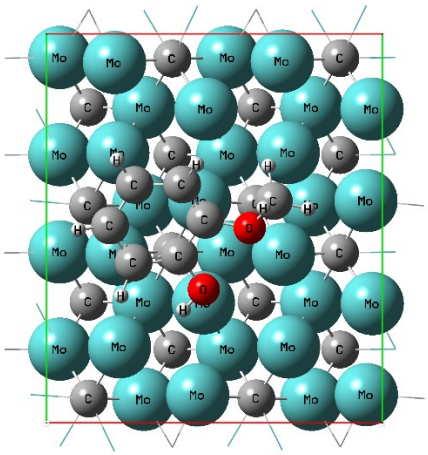
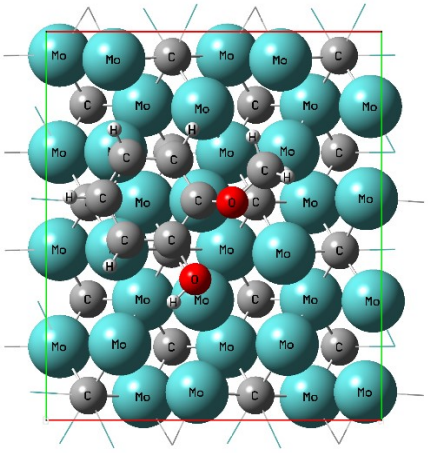
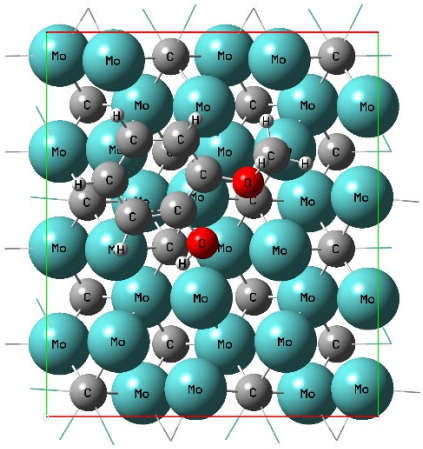
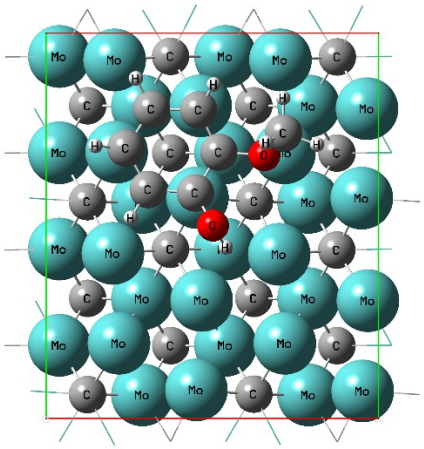
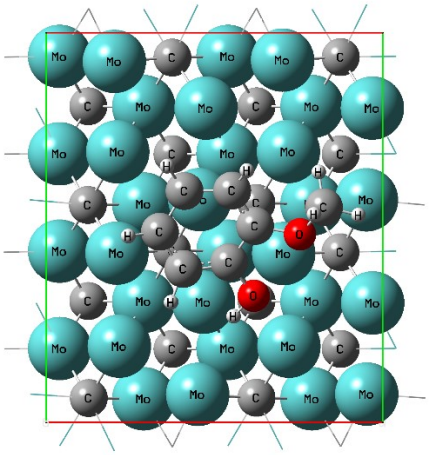
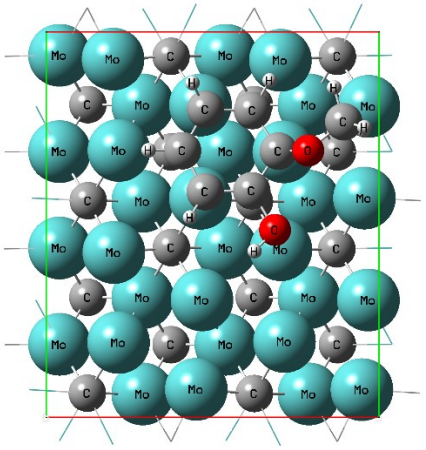
Mo-*hcp*			-4.66
fcc			-4.60

Table S2: Initial and final geometries of the adsorption of guaiacol via the *hydroxyl* group facing the surface at *atop*, *bridge*, C-*hcp*, Mo-*hcp* and *fcc* positions along with their respective adsorption energies (E_{ads}); the atoms are represented as: grey (Carbon), white (hydrogen), red (oxygen) and teal (molybdenum)

	Initial geometry	Final geometry	E_{ads} (eV)
atop			-4.17
bridge			-4.50
C-*hcp*			-4.66

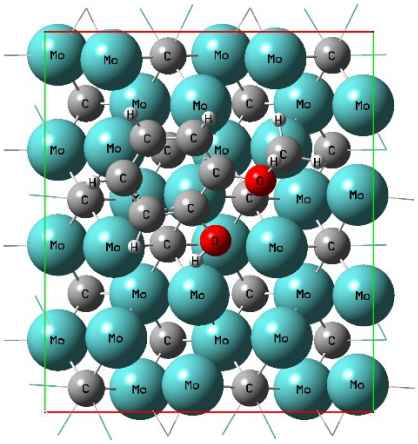
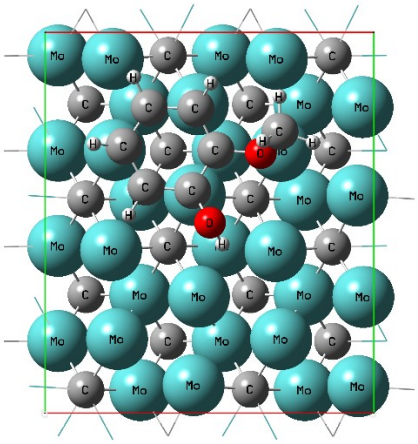
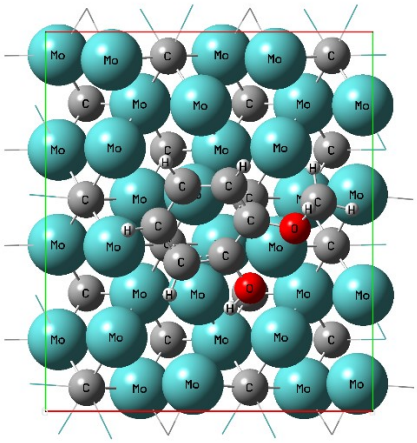
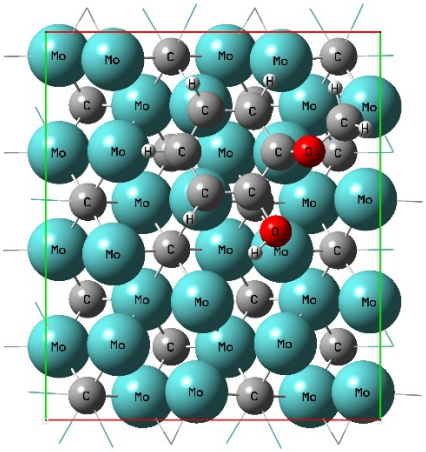
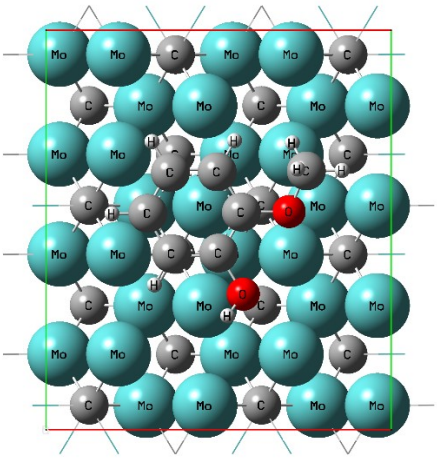
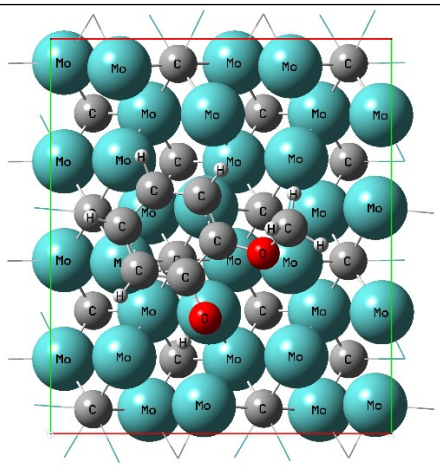
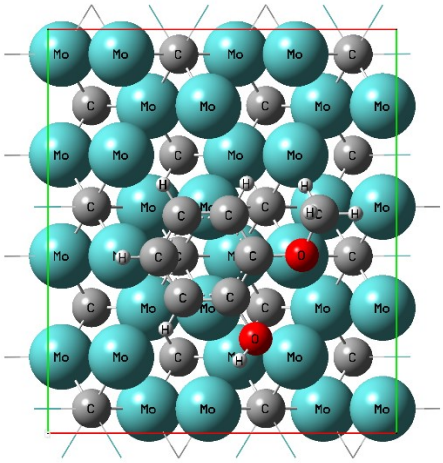
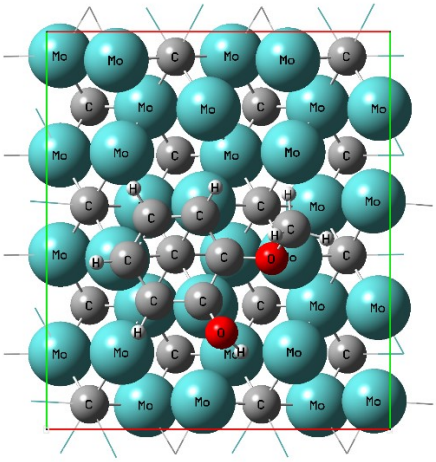
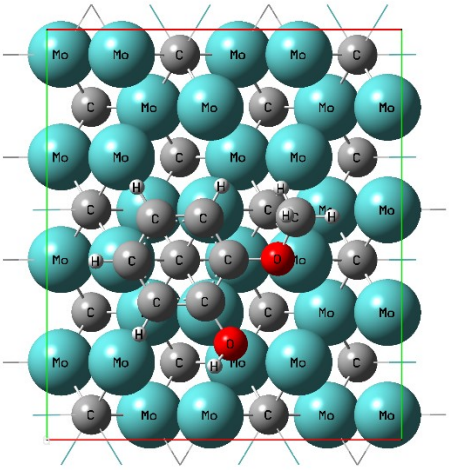
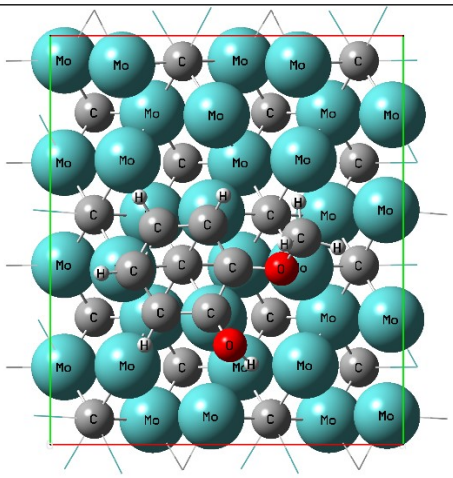
Mo-*hcp*			-4.50
fcc			-4.66

Table S3: Initial and final geometries of the adsorption of guaiacol via the aromatic *ring* facing the surface at *atop*, *bridge*, C-*hcp*, Mo-*hcp* and *fcc* positions along with their respective adsorption energies (E_{ads}); the atoms are represented as: grey (Carbon), white (hydrogen), red (oxygen) and teal (molybdenum)

	Initial geometry	Final geometry	E_{ads} (eV)
atop			-4.09
bridge			-4.67
C-*hcp*			-4.67

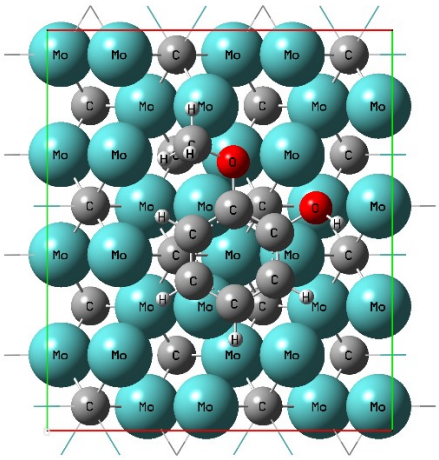
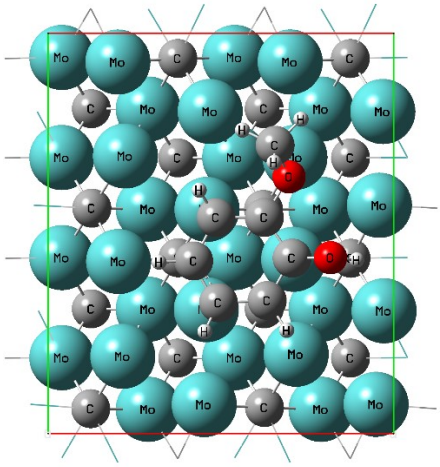
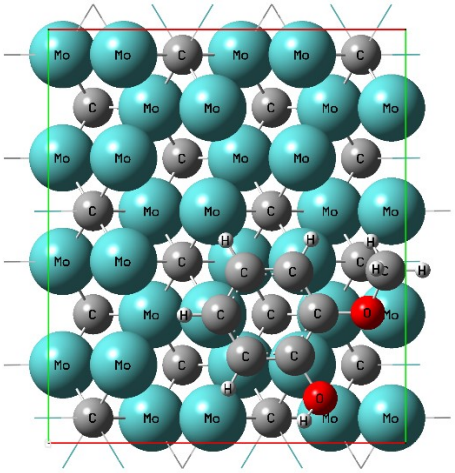
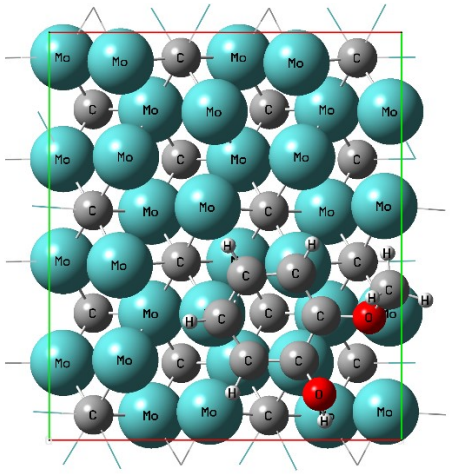
Mo-*hcp*			-4.26
fcc			-4.49

Table S4: All reactions considered in the microkinetic modelling with activation energy (E_a) in eV, reaction energy (ΔE) in eV, activation free energy ($\Delta G^{\ddagger}$) in eV, Arrhenius factor (A_0) and the rate constant (k) in s^{-1} at 500 K, 600 K and 700 K

No.	Reactions	E_a	ΔE	500 K			600 K			700 K		
				$\Delta G^{\ddagger}$	A_0	k	$\Delta G^{\ddagger}$	A_0	k	$\Delta G^{\ddagger}$	A_0	k
R0	GUA + * >> GUA*	-	-4.66	-0.05	1.30E+04	4.19E-03	-0.04	1.18E+04	4.46E-04	-0.04	1.10E+04	6.45E-05
	GUA* >> GUA + *	-	4.66	3.42	2.18E+25	5.21E+00	3.15	1.93E+25	3.75E+02	2.89	1.68E+25	2.67E+04
R1	GUA* + H* >> 1r + *	-	0.25	0.26	1.67E+13	2.35E+11	0.25	1.73E+13	2.64E+11	0.25	1.80E+13	2.99E+11
	1r + * >> GUA* + H*	-	-0.25	-0.26	1.28E+13	9.07E+14	-0.25	1.23E+13	8.06E+14	-0.25	1.18E+13	7.11E+14
	1r > TS1 > 1p	1.15	0.64	1.17	4.47E+13	1.78E+05	1.16	4.46E+13	2.15E+05	1.15	4.39E+13	2.50E+05
	1p > TS1 > 1r	0.5	-0.64	0.44	6.20E+13	4.18E+10	0.43	6.65E+13	5.26E+10	0.42	7.01E+13	6.53E+10
R2	GUA* + H* >> 2r *+ *	-	0.31	0.33	1.01E+13	3.96E+10	0.33	1.02E+13	4.10E+10	0.33	1.04E+13	4.29E+10
	2r* + * >> GUA* + H*	-	-0.31	-0.33	2.12E+13	5.37E+15	-0.33	2.09E+13	5.19E+15	-0.33	2.04E+13	4.96E+15
	2r* > TS2 > 2p*	2.59	0.86	2.45	8.18E+13	1.78E-04	2.44	9.37E+13	2.35E-04	2.43	1.05E+14	3.13E-04
	2p* > TS2 > 2r*	1.73	-0.86	1.55	7.90E+13	5.44E+02	1.55	9.40E+13	7.06E+02	1.54	1.09E+14	9.46E+02
R3	GUA* > TS3 > 3p*	1.04	-0.69	0.96	4.03E+13	4.82E+06	0.95	4.69E+13	6.33E+06	0.95	5.34E+13	8.36E+06
	3p* > TS3 > GUA*	1.73	0.69	1.66	6.68E+13	7.72E+01	1.65	7.42E+13	1.02E+02	1.64	8.06E+13	1.34E+02
	3p* + * >> s4* + OH*	-	-0.37	-0.34	5.59E+12	1.47E+15	-0.32	4.79E+12	1.05E+15	-0.31	4.20E+12	7.46E+14
	s4* + OH* >> 3p* + *	-	0.37	0.34	3.81E+13	1.45E+11	0.32	4.44E+13	2.03E+11	0.31	5.07E+13	2.85E+11
R4	GUA* > TS4 > 4p*	0.90	0.59	0.82	7.62E+13	9.65E+07	0.81	8.67E+13	1.32E+08	0.80	9.60E+13	1.79E+08
	4p* > TS4 > GUA*	0.31	-0.59	0.27	2.45E+13	2.62E+11	0.27	2.55E+13	2.84E+11	0.27	2.63E+13	3.07E+11
	4p* + * >> s5* + OCH3*	-	-1.93	-1.93	3.81E+11	3.17E+25	-1.88	2.48E+11	9.06E+24	-1.83	1.72E+11	2.72E+24
	s5* + OCH3* >> 4p* + *	-	1.93	1.93	5.59E+14	6.70E+00	1.88	8.57E+14	2.35E+01	1.83	1.24E+15	7.83E+01
R5	GUA* > TS5 > 5p*	1.02	-0.49	0.91	2.26E+13	6.76E+06	0.91	2.47E+13	7.09E+06	0.91	2.70E+13	7.78E+06
	5p* > TS5 > GUA*	1.51	0.49	1.47	7.22E+13	1.83E+03	1.46	7.95E+13	2.49E+03	1.45	8.53E+13	3.31E+03
	5p* + * >> s6* + H*	-	-0.14	-0.32	8.89E+11	1.85E+14	-0.24	4.08E+11	2.05E+13	-0.15	1.92E+11	2.24E+12
	s6* + H* >> 5p *	-	0.14	0.32	2.39E+14	1.15E+12	0.24	5.21E+14	1.04E+13	0.15	1.11E+15	9.51E+13
R6	GUA* > TS6 > 6p*	1.44	-2.29	1.25	1.41E+15	1.33E+06	1.22	2.09E+15	3.51E+06	1.18	2.87E+15	9.13E+06
	6p* > TS6 > GUA*	3.73	2.29	3.62	2.23E+15	2.08E-11	3.58	3.02E+15	5.48E-11	3.53	3.80E+15	1.38E-10

	6p* + * >> s7* + CH3*	-	0.07	0.09	7.78E+12	1.65E+12	0.10	6.82E+12	1.24E+12	0.11	6.06E+12	9.34E+11
	s7* + CH3* >> 6p* +*	-	-0.07	-0.09	2.73E+13	1.29E+14	-0.10	3.12E+13	1.71E+14	-0.11	3.51E+13	2.28E+14
R7	GUA* > TS7 > 7p*	0.62	-0.65	0.52	1.21E+13	2.01E+09	0.54	1.13E+13	1.56E+09	0.55	1.07E+13	1.24E+09
	7p* > TS7 > GUA*	1.27	0.65	1.23	2.54E+13	3.69E+04	1.23	2.64E+13	3.83E+04	1.23	2.69E+13	3.94E+04
	7p* + * >> s8*+ H*	-	-0.36	-0.38	1.49E+13	8.10E+15	-0.38	1.43E+13	7.27E+15	-0.37	1.38E+13	6.54E+15
	s8* + H* >> 7p+ *	-	0.36	0.38	1.43E+13	2.63E+10	0.38	1.48E+13	2.93E+10	0.37	1.54E+13	3.26E+10
R8	1p* > TS8 > 8p*	0.75	-0.46	0.67	2.83E+13	4.32E+08	0.67	2.93E+13	4.59E+08	0.66	3.03E+13	4.98E+08
	8p* > TS8 > 1p*	1.21	0.46	1.19	1.41E+14	3.78E+05	1.17	1.51E+14	5.62E+05	1.15	1.56E+14	7.90E+05
	8p* + * >> s9* +H*	-	-0.12	-0.15	2.15E+13	2.71E+14	-0.15	2.18E+13	2.70E+14	-0.15	2.17E+13	2.64E+14
	s9* + H* >> 8p*+ *	-	0.12	0.15	9.89E+12	7.85E+11	0.15	9.77E+12	7.89E+11	0.15	9.79E+12	8.05E+11
R9	1p* > TS9 > 9p*	0.37	-2.05	0.26	2.77E+14	3.68E+12	0.24	3.31E+14	6.24E+12	0.22	3.79E+14	1.04E+13
	9p* > TS9 > 1p*	2.42	2.05	2.38	4.46E+13	3.28E-04	2.37	4.49E+13	3.73E-04	2.37	4.51E+13	4.23E-04
	9p* + * >> s26* + OCH3*	-	-0.5	-0.46	1.15E+11	2.26E+14	-0.40	7.06E+10	5.33E+13	-0.34	4.67E+10	1.34E+13
	s26* + OCH3* >> 9p*+ *	-	0.5	0.46	1.85E+15	9.43E+11	0.40	3.01E+15	3.99E+12	0.34	4.56E+15	1.59E+13
R10	2p* >> 10p*	-	-2.16	-2.16	2.68E+13	9.58E+28	-2.17	3.04E+13	1.23E+29	-2.18	3.37E+13	1.58E+29
	10p* >> 2p*	-	2.16	2.16	7.94E+12	2.22E-03	2.17	7.01E+12	1.73E-03	2.18	6.31E+12	1.34E-03
	10p* + * >> s11* +OH*	-	-0.4	-0.35	3.48E+12	1.12E+15	-0.33	2.96E+12	7.47E+14	-0.32	2.58E+12	5.02E+14
	s11 + OH* >> 10p+ *	-	0.4	0.35	6.12E+13	1.91E+11	0.33	7.18E+13	2.85E+11	0.32	8.24E+13	4.24E+11
R11	s4+ H* >> 11r+ *	-	-0.04	-0.03	1.58E+13	2.48E+13	-0.03	1.65E+13	2.81E+13	-0.04	1.74E+13	3.20E+13
	11r* + * >> s4*+ H*	-	0.04	0.03	1.35E+13	8.56E+12	0.03	1.29E+13	7.58E+12	0.04	1.22E+13	6.65E+12
	11r* > TS11 > 11p*	0.97	-0.29	0.91	7.06E+13	2.13E+07	0.89	8.24E+13	3.07E+07	0.88	9.31E+13	4.33E+07
	11p* > TS11 > 11r*	1.26	0.29	1.12	5.50E+13	4.94E+05	1.11	6.42E+13	6.22E+05	1.11	7.34E+13	7.95E+05
R12	s5* + H* >> 12r +*	-	-0.02	-0.02	1.60E+13	2.07E+13	-0.02	1.68E+13	2.36E+13	-0.03	1.78E+13	2.71E+13
	12r* +* >> s5* +H*	-	0.02	0.02	1.33E+13	1.03E+13	0.02	1.26E+13	9.03E+12	0.03	1.20E+13	7.86E+12
	12r* > TS12 > s26*	1.16	-0.29	1.10	6.48E+13	7.57E+05	1.09	7.50E+13	1.08E+06	1.08	8.38E+13	1.49E+06
	s26* > TS12 > 12r*	1.45	0.29	1.29	1.43E+14	7.28E+04	1.28	1.77E+14	1.11E+05	1.26	2.11E+14	1.70E+05
R13	13r* > TS13 > 13p*	0.79	-0.22	0.88	1.86E+15	8.08E+08	0.79	4.53E+15	9.85E+09	0.69	1.04E+16	1.19E+11
	13p* > TS13 > 13r*	1.01	0.22	0.95	1.31E+14	2.06E+07	0.93	1.47E+14	3.02E+07	0.91	1.60E+14	4.34E+07
	13p * + * >> s5* +OCH2*	-	-0.78	-0.78	1.04E+13	4.50E+18	-0.77	9.21E+12	3.46E+18	-0.77	8.24E+12	2.65E+18
	s5* +OCH2* >> 13p*+ *	-	0.78	0.78	2.05E+13	4.73E+07	0.77	2.31E+13	6.15E+07	0.77	2.58E+13	8.02E+07

R14	14r* > TS14 > 14p*	0.82	-1.58	0.86	5.70E+14	3.63E+08	0.78	1.24E+15	3.05E+09	0.69	2.64E+15	2.63E+10
	14p* > TS14 > 14r*	2.4	1.58	2.33	1.44E+14	2.50E-03	2.31	1.63E+14	3.77E-03	2.29	1.79E+14	5.51E-03
	14p*+ * >> s12*+ H*	-	0.14	0.14	1.31E+13	1.39E+12	0.14	1.23E+13	1.21E+12	0.15	1.16E+13	1.04E+12
	s12*+ H* >> 14p*+ *	-	-0.14	-0.14	1.63E+13	1.53E+14	-0.14	1.73E+13	1.76E+14	-0.15	1.84E+13	2.04E+14
R15	15r* > TS15 > 15p*	0.49	-2.08	0.61	5.63E+14	2.43E+10	0.52	1.20E+15	2.16E+11	0.43	2.48E+15	1.92E+12
	15p* > TS15 > 15r*	2.57	2.08	2.59	1.96E+13	4.78E-06	2.58	1.76E+13	4.34E-06	2.58	1.60E+13	3.95E-06
	15p* + * >> s7*+ CH2*	-	0.08	0.10	7.86E+12	1.53E+12	0.11	6.91E+12	1.16E+12	0.12	6.15E+12	8.82E+11
	s7* + CH2* >> 15p*+ *	-	-0.08	-0.10	2.71E+13	1.39E+14	-0.11	3.08E+13	1.83E+14	-0.12	3.46E+13	2.41E+14
R16	s7* + H* >> 16r* + *	-	-0.03	-0.03	1.47E+13	2.23E+13	-0.03	1.54E+13	2.49E+13	-0.03	1.62E+13	2.83E+13
	16r* + * >> s7* +H*	-	0.03	0.03	1.45E+13	9.56E+12	0.03	1.38E+13	8.53E+12	0.03	1.31E+13	7.53E+12
	16r* > TS16 > 16p*	1.81	1.43	1.71	1.94E+14	8.80E+01	1.70	2.30E+14	1.43E+02	1.68	2.61E+14	2.27E+02
	16p* > TS16 > 16r*	0.38	-1.43	0.22	1.17E+14	3.13E+12	0.21	1.31E+14	4.06E+12	0.20	1.44E+14	5.37E+12
R17	s7* + H* >> 17r*+ *	-	0.54	0.58	1.14E+13	7.98E+08	0.57	1.15E+13	8.43E+08	0.57	1.17E+13	8.92E+08
	17r* + * >> s7* +H*	-	-0.54	-0.58	1.86E+13	2.67E+17	-0.57	1.85E+13	2.52E+17	-0.57	1.82E+13	2.39E+17
	17r* > TS17 > 17p*	2.46	0.52	2.37	1.32E+13	1.11E-04	2.38	1.33E+13	9.74E-05	2.39	1.33E+13	8.60E-05
	17p* > TS17 > 17r*	1.95	-0.52	1.77	2.47E+13	4.31E+00	1.78	2.71E+13	4.17E+00	1.79	2.92E+13	4.11E+00
R18	18r* > TS18 > 18p*	1.03	-1.19	0.94	8.30E+13	1.44E+07	0.93	9.39E+13	2.00E+07	0.91	1.04E+14	2.80E+07
	18p* > TS18 > 18r*	2.22	1.19	2.13	2.32E+14	1.03E-01	2.11	2.59E+14	1.62E-01	2.09	2.82E+14	2.49E-01
	18p* + * >> s15* +OH*	-	0.22	0.24	8.64E+12	1.57E+11	0.25	7.68E+12	1.22E+11	0.26	6.90E+12	9.43E+10
	s15* + OH* >> 18p* +*	-	-0.22	-0.24	2.46E+13	1.36E+15	-0.25	2.77E+13	1.75E+15	-0.26	3.08E+13	2.26E+15
R19	19r* > TS19 > 19p*	0.39	-1.99	0.29	7.42E+13	5.60E+11	0.28	8.75E+13	7.82E+11	0.27	1.00E+14	1.09E+12
	19p* > TS19 > 19r*	2.38	1.99	2.32	6.00E+13	1.23E-03	2.31	6.52E+13	1.56E-03	2.30	6.96E+13	1.97E-03
	19p* + * >> s15* +OCH3*	-	0.4	0.41	3.43E+11	3.98E+08	0.46	2.19E+11	1.10E+08	0.51	1.49E+11	3.18E+07
	s15* + OCH3* >> 19p* +*	-	-0.4	-0.41	6.20E+14	5.34E+17	-0.46	9.72E+14	1.94E+18	-0.51	1.43E+15	6.69E+18
R20	20r* > TS20 > 20p*	0.78	-0.54	0.65	3.66E+13	7.88E+08	0.65	4.12E+13	9.15E+08	0.64	4.59E+13	1.10E+09
	20p* > TS20 > 20r*	1.32	0.54	1.25	1.83E+14	1.78E+05	1.23	2.12E+14	2.89E+05	1.21	2.35E+14	4.54E+05
	20p* + * >> s12* +H*	-	-0.53	-0.53	1.02E+13	7.03E+16	-0.53	9.91E+12	6.08E+16	-0.52	9.57E+12	5.26E+16
	s12* + H* >> 20p* +*	-	0.53	0.53	2.08E+13	3.03E+09	0.53	2.15E+13	3.50E+09	0.52	2.22E+13	4.04E+09
R21	21r* >> 21p*	-	-1.94	-1.99	1.06E+13	2.45E+27	-1.99	1.15E+13	2.49E+27	-1.99	1.23E+13	2.57E+27
	21p* >> 21r*	-	1.94	1.99	2.00E+13	8.70E-02	1.99	1.86E+13	8.55E-02	1.99	1.73E+13	8.29E-02

	21p* + * >> s17* +CH2*	-	-0.03	-0.02	1.35E+13	1.82E+13	-0.01	1.26E+13	1.59E+13	-0.01	1.18E+13	1.38E+13
	s17* + CH2* >> 21p* +*	-	0.03	0.02	1.58E+13	1.17E+13	0.01	1.69E+13	1.34E+13	0.01	1.81E+13	1.54E+13
R22	11p* > TS22 > 22p*	1.02	-0.52	0.90	2.57E+13	8.67E+06	0.90	2.85E+13	9.34E+06	0.90	3.14E+13	1.05E+07
	22p* > TS22 > 11p*	1.54	0.52	1.50	7.36E+13	1.17E+03	1.49	8.19E+13	1.61E+03	1.47	8.87E+13	2.16E+03
	22p* + * >> s18*+ H*	-	-0.15	-0.18	1.67E+13	3.21E+14	-0.17	1.66E+13	3.01E+14	-0.17	1.63E+13	2.81E+14
	s18* + H* >> 22p* +*	-	0.15	0.18	1.27E+13	6.64E+11	0.17	1.28E+13	7.06E+11	0.17	1.30E+13	7.58E+11
R23	23r* >> 23p*	-	-2.05	-2.11	2.00E+13	2.97E+28	-2.11	2.18E+13	3.33E+28	-2.11	2.35E+13	3.73E+28
	23p* >> 23r*	-	2.05	2.11	1.06E+13	7.17E-03	2.11	9.74E+12	6.40E-03	2.11	9.04E+12	5.70E-03
	23p* + * >> s19*+ CH2*	-	0.07	0.09	7.96E+12	1.72E+12	0.10	7.02E+12	1.32E+12	0.11	6.27E+12	1.00E+12
	s19* + OCH3* >> 19p*+ *	-	-0.07	-0.09	2.67E+13	1.23E+14	-0.10	3.03E+13	1.62E+14	-0.11	3.39E+13	2.12E+14
R24	16p* > TS24 > 24p*	0.18	-1.12	0.11	6.01E+13	9.12E+12	0.10	6.83E+13	1.22E+13	0.09	7.60E+13	1.65E+13
	24p* > TS24 > 16p*	1.3	1.12	1.26	4.89E+13	4.36E+04	1.25	5.12E+13	5.17E+04	1.24	5.30E+13	6.12E+04
	24p* + * >> s5* +OH*	-	0.01	0.03	8.68E+12	5.15E+12	0.04	7.67E+12	3.97E+12	0.05	6.86E+12	3.06E+12
	s5* + OH* >> 24p* +*	-	-0.01	-0.03	2.45E+13	4.13E+13	-0.04	2.77E+13	5.36E+13	-0.05	3.10E+13	6.96E+13
R25	16p* + H* >> 25r* +*	-	0.44	0.47	1.34E+13	5.48E+09	0.47	1.36E+13	5.93E+09	0.46	1.38E+13	6.42E+09
	25r* + * >> 16p* +H*	-	-0.44	-0.47	1.59E+13	3.88E+16	-0.47	1.57E+13	3.59E+16	-0.46	1.54E+13	3.31E+16
	25r* >> 25p*	-	2.98	2.91	1.58E+13	1.73E-08	2.92	1.55E+13	1.54E-08	2.92	1.52E+13	1.37E-08
	25p* >> 25r*	-	-2.98	-2.91	1.35E+13	1.23E+34	-2.92	1.37E+13	1.38E+34	-2.92	1.40E+13	1.55E+34
R26	17p* > TS26 > 26p*	0.09	-1.87	0.08	1.64E+13	4.40E+12	0.08	1.68E+13	4.56E+12	0.08	1.71E+13	4.73E+12
	26p* > TS26 > 17p*	1.95	1.87	1.96	1.29E+13	9.27E-02	1.97	1.18E+13	8.16E-02	1.97	1.10E+13	7.16E-02
	26p* + * >> s19*+ OH*	-	-0.6	-0.59	8.69E+12	1.53E+17	-0.58	7.94E+12	1.22E+17	-0.57	7.30E+12	9.75E+16
	s19* + OH* >> 26p*+ *	-	0.6	0.59	2.45E+13	1.39E+09	0.58	2.68E+13	1.74E+09	0.57	2.91E+13	2.18E+09
R27	s15* + H* >> 27r* +*	-	-0.66	-0.65	1.22E+13	5.80E+17	-0.65	1.27E+13	6.35E+17	-0.66	1.34E+13	7.06E+17
	27r* + * >> s15* +H*	-	0.66	0.65	1.74E+13	3.67E+08	0.65	1.67E+13	3.35E+08	0.66	1.59E+13	3.01E+08
	27r* > TS27 > s19*	1.15	0.23	1.09	7.30E+13	9.72E+05	1.08	8.63E+13	1.44E+06	1.07	9.81E+13	2.07E+06
	s19* > TS27 > 27r*	0.92	-0.23	0.79	4.09E+13	8.27E+07	0.79	4.83E+13	1.03E+08	0.78	5.56E+13	1.29E+08
R28	28r* >> 28p*	-	-2.31	-2.38	1.87E+13	2.54E+30	-2.38	2.09E+13	2.86E+30	-2.38	2.30E+13	3.23E+30
	28p* >> 28r*	-	2.31	2.38	1.14E+13	8.39E-05	2.38	1.02E+13	7.45E-05	2.38	9.25E+12	6.59E-05
	28p*+ * >> s23* +CH2*	-	0.06	0.08	7.75E+12	1.91E+12	0.09	6.83E+12	1.45E+12	0.10	6.10E+12	1.10E+12
	s23* + CH2* >> 28p* +*	-	-0.06	-0.08	2.74E+13	1.11E+14	-0.09	3.11E+13	1.46E+14	-0.10	3.49E+13	1.93E+14

R29	s17* + H* >> 29r* +*	-	0.23	0.24	1.19E+13	2.25E+11	0.24	1.24E+13	2.42E+11	0.23	1.29E+13	2.64E+11
	29r* + * >> s17*+ H*	-	-0.23	-0.24	1.78E+13	9.43E+14	-0.24	1.72E+13	8.80E+14	-0.23	1.65E+13	8.07E+14
	29r* > TS29 > 25p*	1.22	3.61	1.16	1.07E+14	5.05E+05	1.14	1.20E+14	7.15E+05	1.13	1.30E+14	9.89E+05
	25p* > TS29 > 29r*	-2.39	-3.61	-2.39	2.92E+13	4.98E+30	-2.40	3.08E+13	6.04E+30	-2.41	3.24E+13	7.38E+30
R30	s19* + H* >> 30r* +*	-	-0.03	-0.02	1.50E+13	2.19E+13	-0.03	1.57E+13	2.46E+13	-0.03	1.65E+13	2.79E+13
	30r* + * >> s19* +H*	-	0.03	0.02	1.42E+13	9.72E+12	0.03	1.35E+13	8.66E+12	0.03	1.29E+13	7.63E+12
	30r* > TS30 > s26*	2.19	1.41	2.12	5.97E+13	3.00E-02	2.11	6.86E+13	4.11E-02	2.10	7.64E+13	5.54E-02
	s26* > TS30 > 30r*	0.78	-1.41	0.65	3.19E+13	6.73E+08	0.65	3.46E+13	7.20E+08	0.65	3.74E+13	7.91E+08
R31	25p* >> 31p*	-	-4.47	-4.36	1.96E+13	4.79E+44	-4.37	2.19E+13	6.78E+44	-4.39	2.40E+13	9.44E+44
	31p* >> 25p*	-	4.47	4.36	1.08E+13	4.44E-19	4.37	9.72E+12	3.14E-19	4.39	8.85E+12	2.25E-19
	31p*+ * >> s26* +OH*	-	-0.39	-0.34	3.97E+12	1.09E+15	-0.33	3.37E+12	7.39E+14	-0.31	2.93E+12	5.02E+14
	s26* + OH* >> 31p*+ *	-	0.39	0.34	5.35E+13	1.95E+11	0.33	6.31E+13	2.88E+11	0.31	7.27E+13	4.24E+11
R32	s23*+ H* >> 32r*+ *	-	-0.01	0.00	1.54E+13	1.57E+13	-0.01	1.62E+13	1.78E+13	-0.01	1.70E+13	2.03E+13
	32r*+ * >> s23*+ H*	-	0.01	0.00	1.38E+13	1.35E+13	0.01	1.32E+13	1.20E+13	0.01	1.25E+13	1.05E+13
	32r* > TS32 > s7*	2.28	1.69	2.19	1.89E+14	2.99E-02	2.17	2.25E+14	4.95E-02	2.15	2.58E+14	7.98E-02
	s7* > TS32 > 32r*	0.58	-1.69	0.45	3.11E+13	1.91E+10	0.45	3.32E+13	2.00E+10	0.45	3.55E+13	2.16E+10
R33	s26* > TS33 > 33p*	1.5	-0.73	1.40	7.27E+13	6.05E+03	1.39	8.62E+13	8.53E+03	1.38	9.91E+13	1.20E+04
	33p* > TS33 > s26*	2.23	0.73	2.15	9.99E+13	3.06E-02	2.14	1.12E+14	4.26E-02	2.13	1.22E+14	5.82E-02
	33p* + * >> s25*+ OH*	-	-0.11	-0.09	9.14E+12	4.20E+13	-0.08	8.14E+12	3.28E+13	-0.08	7.32E+12	2.56E+13
	s25* + OH* >> 33p*+ *	-	0.11	0.09	2.33E+13	5.06E+12	0.08	2.61E+13	6.48E+12	0.08	2.91E+13	8.32E+12
R34	s26*+ H* >> 34r*+ *	-	0.9	0.89	3.53E+13	1.30E+07	0.88	3.72E+13	1.64E+07	0.87	3.90E+13	2.06E+07
	34r* + * >> s26*+ H*	-	-0.9	-0.89	6.03E+12	1.63E+19	-0.88	5.72E+12	1.29E+19	-0.87	5.46E+12	1.03E+19
	34r* > TS34 > 34p*	2.06	0.57	1.88	1.66E+14	5.05E+00	1.86	1.98E+14	7.46E+00	1.85	2.29E+14	1.12E+01
	34p* > TS34 > 34r*	1.49	-0.57	1.21	3.45E+14	6.53E+05	1.20	4.54E+14	1.09E+06	1.18	5.76E+14	1.90E+06
R35	s25* + H* >> 35r* +*	-	0.48	0.46	2.83E+13	1.33E+10	0.45	3.04E+13	1.64E+10	0.45	3.26E+13	2.04E+10
	35r* + * >> s25*+ H*	-	-0.48	-0.46	7.52E+12	1.60E+16	-0.45	6.99E+12	1.29E+16	-0.45	6.52E+12	1.04E+16
	35r* > TS35 > 35p*	0.75	-0.5	0.69	5.26E+13	5.33E+08	0.68	6.09E+13	7.34E+08	0.67	6.81E+13	9.88E+08
	35p* > TS35 > 35r*	1.25	0.5	1.10	3.70E+13	4.16E+05	1.10	4.31E+13	4.96E+05	1.10	4.93E+13	6.02E+05
R36	34p* > TS36 > 36p*	0.5	-1.94	0.48	1.83E+13	6.63E+09	0.48	1.84E+13	6.39E+09	0.48	1.84E+13	6.17E+09
	36p* > TS36 > 34p*	2.45	1.94	2.49	4.58E+12	5.20E-06	2.51	3.70E+12	3.33E-06	2.52	3.07E+12	2.14E-06

	34p* + * >> s29* +OH*	-	-2.33	-2.35	1.60E+13	1.42E+30	-2.35	1.69E+13	1.44E+30	-2.35	1.75E+13	1.47E+30
	s29* + OH* >> 34p* +*	-	2.33	2.35	1.33E+13	1.50E-04	2.35	1.26E+13	1.48E-04	2.35	1.21E+13	1.45E-04
R37	CH2*+ H* >> 37r+ *	-	0.28	0.27	1.85E+13	2.04E+11	0.27	2.01E+13	2.44E+11	0.26	2.17E+13	2.96E+11
	37r* + * >> CH2*+ H*	-	-0.28	-0.27	1.15E+13	1.04E+15	-0.27	1.06E+13	8.71E+14	-0.26	9.79E+12	7.19E+14
	37r* > TS37 > CH3*	0.72	0.14	0.73	1.90E+13	1.08E+08	0.72	1.92E+13	1.16E+08	0.72	1.93E+13	1.22E+08
	CH3* > TS37 > 37r*	0.58	-0.14	0.50	2.11E+13	5.22E+09	0.50	2.30E+13	5.64E+09	0.50	2.48E+13	6.21E+09
R38	CH3* + H* >> 38r* +*	-	0.49	0.50	1.81E+13	4.65E+09	0.49	1.95E+13	5.62E+09	0.48	2.10E+13	6.78E+09
	38r* + * >> CH3*+ H*	-	-0.49	-0.50	1.17E+13	4.57E+16	-0.49	1.09E+13	3.79E+16	-0.48	1.01E+13	3.14E+16
	38r* > TS38 > CH4*	1.56	1.25	1.53	7.62E+13	7.04E+02	1.52	8.21E+13	9.37E+02	1.51	8.62E+13	1.21E+03
	CH4* > TS38 > 38r*	0.3	-1.25	0.27	8.31E+11	9.00E+09	0.30	7.63E+11	5.19E+09	0.33	7.30E+11	3.19E+09
R39	OH* + H* >> 39r* +*	-	0.02	0.02	1.61E+13	1.09E+13	0.02	1.70E+13	1.25E+13	0.01	1.80E+13	1.44E+13
	39r + * >> OH*+H*	-	-0.02	-0.02	1.32E+13	1.95E+13	-0.02	1.25E+13	1.70E+13	-0.01	1.18E+13	1.47E+13
	39r > TS39 > H2O*	2.15	1.65	2.07	9.33E+13	1.10E-01	2.06	1.08E+14	1.58E-01	2.05	1.21E+14	2.25E-01
	H2O* > TS39 > 39r*	0.5	-1.65	0.39	1.29E+13	2.09E+10	0.40	1.34E+13	1.90E+10	0.40	1.41E+13	1.81E+10
R40	OCH2* H* >> 40r *	-	0.11	0.12	1.68E+13	2.47E+12	0.11	1.80E+13	2.89E+12	0.10	1.93E+13	3.42E+12
	40r*+ * >> OCH2*+ H*	-	-0.11	-0.12	1.27E+13	8.61E+13	-0.11	1.18E+13	7.36E+13	-0.10	1.10E+13	6.23E+13
	40r* > TS40 > OCH3*	0.85	0.17	0.85	5.36E+13	3.87E+07	0.84	5.91E+13	5.33E+07	0.83	6.32E+13	7.04E+07
	OCH3* > TS40 > 40r*	0.68	-0.17	0.62	1.46E+14	4.63E+09	0.59	2.12E+14	1.13E+10	0.56	2.95E+14	2.73E+10
R41	OCH3* H* >> 41r *	-	-0.01	0.04	1.51E+14	7.24E+13	0.00	2.07E+14	1.93E+14	-0.04	2.73E+14	4.94E+14
	41r* + * >> OCH3* +H*	-	0.01	-0.04	1.41E+12	2.94E+12	0.00	1.03E+12	1.10E+12	0.04	7.79E+11	4.30E+11
	41r* > TS41 > CH3OH*	2.45	2.14	2.33	3.77E+14	6.27E-03	2.31	4.75E+14	1.17E-02	2.28	5.66E+14	2.14E-02
	CH3OH* > TS41 > 41r*	0.31	-2.14	0.15	7.10E+13	5.58E+12	0.15	8.07E+13	6.91E+12	0.14	9.02E+13	8.74E+12
R42	s26* >> phenol+ *	-	4.45	3.25	8.91E+24	3.49E+01	3.00	8.24E+24	2.25E+03	2.74	7.41E+24	1.43E+05
	phenol + * >> s26*	-	-4.45	-0.05	1.26E+04	1.84E-01	-0.04	1.26E+04	4.81E-02	-0.04	1.26E+04	1.42E-02
R43	16p* >> catechol +*	-	4.26	3.08	9.24E+24	6.63E+02	2.82	8.24E+24	4.40E+04	2.56	7.20E+24	2.87E+06
	catechol + * >> 16p*	-	-4.26	-0.04	1.16E+04	3.01E-02	-0.03	1.16E+04	6.39E-03	-0.03	1.16E+04	1.58E-03
R44	s29* >> benzene +*	-	4.06	3.09	2.18E+22	1.18E+00	2.90	1.79E+22	2.54E+01	2.70	1.46E+22	5.49E+02
	benzene + * >> s29*	-	-4.06	-0.07	1.38E+04	1.22E+00	-0.06	1.38E+04	3.92E-01	-0.05	1.38E+04	1.38E-01
R45	CH4* >> CH4 +*	-	0.38	-0.37	1.19E+19	5.16E+21	-0.50	1.04E+19	4.18E+22	-0.64	9.06E+18	3.51E+23
	CH4 + * >> CH4*	-	-0.38	-0.07	3.05E+04	2.99E+01	-0.06	3.05E+04	1.82E+01	-0.05	3.05E+04	1.18E+01

R46	CH3OH* >> CH3OH +*	-	1.18	0.16	1.95E+22	1.31E+21	-0.04	1.98E+22	3.82E+22	-0.25	1.94E+22	1.13E+24
	CH3OH + * >> CH3OH*	-	-1.18	-0.05	2.16E+04	5.91E+00	-0.04	2.16E+04	3.20E+00	-0.04	2.16E+04	1.86E+00
R47	H2O* >> H2O+ *	-	1.07	0.25	4.19E+20	6.31E+18	0.08	4.73E+20	1.22E+20	-0.09	5.08E+20	2.33E+21
	H2O + * >> H2O*	-	-1.07	-0.03	2.88E+04	1.63E+01	-0.03	2.88E+04	1.14E+01	-0.03	2.88E+04	8.40E+00
R48	H2* >> H2+ *	-	0.79	0.27	4.91E+18	5.82E+16	0.13	6.88E+18	8.09E+17	-0.01	8.82E+18	1.08E+19
	H2 + * >> H2*	-	-0.79	0.00	8.60E+04	8.51E+01	0.00	8.60E+04	6.47E+01	0.00	8.60E+04	5.14E+01
R49	H* + H* >> 49r*+ *	-	0	0.01	1.57E+13	1.38E+13	0.00	1.64E+13	1.55E+13	0.00	1.72E+13	1.76E+13
	49r* + * >> H* +H*	-	0	-0.01	1.35E+13	1.54E+13	0.00	1.29E+13	1.37E+13	0.00	1.23E+13	1.21E+13
R50	s19* > TS50 > 37p*	1.59	-0.89	1.51	8.27E+13	1.21E+03	1.49	9.67E+13	1.71E+03	1.48	1.10E+14	2.41E+03
	37p* > TS50 > s19*	2.48	0.89	2.42	7.05E+13	2.70E-04	2.41	7.67E+13	3.48E-04	2.40	8.18E+13	4.47E-04
	37p* + * >> s25* +O*	-	0.09	0.10	6.05E+12	1.16E+12	0.11	5.26E+12	8.24E+11	0.12	4.66E+12	5.89E+11
	s25* + O* >> 37p + *	-	-0.09	-0.10	3.51E+13	1.84E+14	-0.11	4.04E+13	2.58E+14	-0.12	4.57E+13	3.61E+14
R51	O* + H* >> 61r* + *	-	0.17	0.18	1.64E+13	8.59E+11	0.17	1.73E+13	9.84E+11	0.17	1.84E+13	1.14E+12
	61r* + * >> O* + H*	-	-0.17	-0.18	1.30E+13	2.48E+14	-0.17	1.23E+13	2.16E+14	-0.17	1.16E+13	1.87E+14
	61r* > TS51 > OH*	1.97	1.16	1.94	3.77E+13	4.39E-01	1.93	4.23E+13	5.61E-01	1.92	4.61E+13	7.02E-01
	OH* > TS51 > 61r*	0.82	-1.16	0.69	2.35E+13	2.41E+08	0.70	2.49E+13	2.42E+08	0.70	2.63E+13	2.48E+08
R52	49r *>> H2*	-	1.46	1.45	3.83E+13	1.39E+03	1.44	4.29E+13	1.87E+03	1.43	4.64E+13	2.41E+03
	H2* >> 49r*	-	-1.46	-1.45	5.55E+12	1.53E+23	-1.44	4.96E+12	1.14E+23	-1.43	4.58E+12	8.82E+22