Microkinetic modelling of HC-SCR of NO to N_2, N_2O and NO_2 on Pt catalysts in automotive aftertreatment

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Table S1. Reaction mechanism and kinetic data for NO reduction using Propene (HC-SCR) on Pt catalysts[9,12,13]

NO.	Reactions	Pre-exponential factor $k_0(s^{-1})$/sticking coefficient	Activation energy E_a (kJ/mol)	References
ADSORPTION				
1	$O_2 + 2* \rightarrow 2O^*$	0.007	0	9
2	$C_3H_6 + 2^* \rightarrow C_3H_6^*$	0.98	0	9
3	$C_3H_6 + O^* + * \rightarrow C_3H_5^* + OH^*$	0.005	0	9
4	$H_2 + 2* \rightarrow 2H^*$	0.046	0	9
5	$H_2O + * \rightarrow H_2O^*$	0.75	0	9
6	$CO_2 + * \rightarrow CO_2^*$	0.005	0	9
7	$CO + * \rightarrow CO^*$	0.84	0	9
8	$NO + * \rightarrow NO^*$	0.85	0	12
9	$N_2O + * \rightarrow N_2O^*$	.025	0	12
10	$NO_2 + * \rightarrow NO_2^*$	.9	0	12
DESORPTION				
11	$2O^* \rightarrow O_2 + 2*$	7.54×10^{12}	232.2	9
12	$C_3H_6^* \rightarrow C_3H_6 + 2^*$	1.0×10^{13}	72.7	9
13	$C_3H_5^* + OH^* \rightarrow C_3H_6 + O^* + *$	7.54×10^{12}	31	9
14	$2H^* \rightarrow H_2 + 2*$	7.54×10^{12}	67.4	9
15	$H_2O^* \rightarrow * + H_2O$	1.0×10^{13}	40.3	9
16	$CO_2^* \rightarrow CO_2 + *$	1.0×10^{13}	27.1	9
17	$CO^* \rightarrow CO + *$	1.0×10^{13}	136.4	9
18	$NO^* \rightarrow NO + *$	1.0×10^{16}	140	12

19	$N_2O^* \rightarrow N_2O + *$	1.0x10^{13}	54.4	[12]
20	$NO_2^* \rightarrow NO_2 + *$	1.0x10^{13}	60.0	[12]
21	$N^* + N^* \rightarrow N_2 + 2*$	4.14x10^{15} #	113.9	[9]
SURFACE REACTION				
22	$C_3H_5^* + 5O^* + 2* \rightarrow 5OH^* + 3C^*$	7.54x10^{12}	95	[9]
23	$C_3H_6^* \rightarrow H^* + CC_2H_5^*$	1.0x10^{13}	75.4	[9]
24	$CC_2H_5^* + H^* \rightarrow C_3H_6^*$	7.54x10^{12}	48.8	[9]
25	$CC_2H_5^* + * \rightarrow C_2H_3^* + CH_2^*$	7.54x10^{12}	108.2	[9]
26	$C_2H_3^* + CH_2^* \rightarrow CC_2H_5^* + *$	7.54x10^{12}	3.2	[9]
27	$C_2H_3^* + * \rightarrow CH_3^* + C^*$	7.54x10^{12}	46	[9]
28	$CH_3^* + C^* \rightarrow C_2H_3^* + *$	7.54x10^{12}	46.9	[9]
29	$CH_3^* + * \rightarrow CH_2^* + H^*$	2.57x10^{13}	70.4	[9]
30	$CH_2^* + H^* \rightarrow CH_3^* + *$	6.30x10^{13}	0	[9]
31	$CH_2^* + * \rightarrow CH^* + H^*$	1.42x10^{14}	59.2	[9]
32	$CH^* + H^* \rightarrow CH_2^* + *$	6.30x10^{13}	0	[9]
33	$CH^* + * \rightarrow C^* + H^*$	6.30x10^{13}	0	[9]
34	$C^* + H^* \rightarrow CH^* + *$	2.55x10^{13}	138	[9]
35	$C_2H_3^* + O^* \rightarrow * + CH_3CO^*$	7.54x10^{10}	62.3	[9]
36	$CH_3CO^* + * \rightarrow C_2H_3^* + O^*$	7.54x10^{12}	196.7	[9]
37	$CH_3^* + CO^* \rightarrow * + CH_3CO^*$	7.54x10^{12}	82.9	[9]
38	$CH_3CO^* + * \rightarrow CH_3^* + CO^*$	7.54x10^{12}	0	[9]
39	$CH_3^* + O^* \rightarrow CH_2^* + OH^*$	7.54x10^{12}	36.6	[9]
40	$CH_2^* + OH^* \rightarrow CH_3^* + O^*$	7.54x10^{12}	25.1	[9]
41	$CH_2^* + O^* \rightarrow CH^* + OH^*$	7.54x10^{12}	25.1	[9]
42	$CH^* + OH^* \rightarrow CH_2^* + O^*$	7.54x10^{12}	25.2	[9]
43	$CH^* + O^* \rightarrow C^* + OH^*$	7.54x10^{12}	25.1	[9]
44	$C^* + OH^* \rightarrow CH^* + O^*$	7.54x10^{12}	224.8	[9]
45	$O^* + H^* \rightarrow OH^* + *$	7.54x10^{12}	11.5	[9]
46	$OH^* + * \rightarrow O^* + H^*$	1.17x10^{14}	74.9	[9]
47	$OH^* + H^* \rightarrow H_2O^* + *$	7.54x10^{12}	17.4	[9]
48	$H_2O^* + * \rightarrow OH^* + H^*$	7.46x10^{12}	73.6	[9]
49	$OH^* + OH^* \rightarrow H_2O^* + O^*$	7.54x10^{12}	48.2	[9]

50	$H_2O^* + O^* \rightarrow OH^* + OH^*$	4.794×10^{11}	41	[9]
51	$CO^* + O^* \rightarrow CO_2^* + *$	7.54×10^{11}	108	[9]
52	$CO_2^* + * \rightarrow CO^* + O^*$	7.54×10^{12}	165.1	[9]
53	$C^* + O^* \rightarrow CO^* + *$	7.54×10^{12}	0	[9]
54	$CO^* + * \rightarrow C^* + O^*$	7.54×10^{12}	218.5	[9]
55	$NO^* + * \rightarrow N^* + O^*$	1.02×10^{12}	107.8	[9]
56	$N^* + O^* \rightarrow NO^* + ^*$	7.54×10^{12}	128.1	[9]
57	$NO^* + N^* \rightarrow N_2O^* + *$	2.04×10^{9} #	90.9	[12]
58	$N_2O^* + * \rightarrow NO^* + N^*$	7.54×10^{12}	66.9	[12]
59	$NO^* + O^* \rightarrow NO_2^* + *$	7.54×10^{12} #	130.6	[13]
60	$NO_2^* + * \rightarrow NO^* + O^*$	7.54×10^{11} #	0.0	[13]

 # assumed (this work).