Table S1 A list of selected H-atom abstraction reactions in the present four hexane isomers sub-mechanism, units are s^{-1}, cm^3 and cal/mol.

No.	Reactions	A	n	E_a	References
R1	$NC_6H_{14} + H = C_6H_{13}\text{-}1 + H_2$	1.170E+08	1.935	7650.0	[1]
R2	$NC_6H_{14} + H = C6H_{13}\text{-}2 + H_2$	1.950E+08	1.840	5266.0	[1]
R3	$NC_6H_{14} + H = C6H_{13}\text{-}3 + H_2$	1.950E+08	1.840	5266.0	[1]
R4	$NC_6H_{14} + CH_3 = C_6H_{13}\text{-}1 + CH_4$	9.060E-01	3.650	7154.0	[2]
R5	$NC_6H_{14} + CH_3 = C_6H_{13}\text{-}2 + CH_4$	3.020E+00	3.460	5481.0	[2]
R6	$NC_6H_{14} + CH_3 = C_6H_{13}\text{-}3 + CH_4$	3.020E+00	3.460	5481.0	[2]
R7	$NC_6H_{14} + OH = C_6H_{13}\text{-}1 + H_2O$	1.760E+09	0.970	1586.0	[3]
R8	$NC_6H_{14} + OH = C_6H_{13}\text{-}2 + H_2O$	2.340E+07	1.610	-35.0	[3]
R9	$NC_6H_{14} + OH = C_6H_{13}\text{-}3 + H_2O$	2.340E+07	1.610	-35.0	[3]
R10	$IC_6 + H = IC_6\text{-}1 + H_2$	1.040E+08	1.943	7898.0	[1]
R11	$IC_6 + H = IC_6\text{-}2 + H_2$	5.700E+07	1.849	3080.0	[1]
R12	$IC_6 + H = IC_6\text{-}3 + H_2$	9.750E+07	1.840	5266.0	[1]
R13	$IC_6 + H = IC_6\text{-}4 + H_2$	9.750E+07	1.840	5266.0	[1]
R14	$IC_6 + H = IC_6\text{-}5 + H_2$	5.850E+07	1.935	7650.0	[1]
R15	$IC_6 + CH_3 = IC_6\text{-}1 + CH_4$	3.600E+00	3.650	7150.0	[4]
R16	$IC_6 + CH_3 = IC_6\text{-}2 + CH_4$	3.600E+00	3.460	4600.0	[4]
R17	$IC_6 + CH_3 = IC_6\text{-}3 + CH_4$	1.510E+00	3.460	5481.0	[2]
R18	$IC_6 + CH_3 = IC_6\text{-}4 + CH_4$	1.510E+00	3.460	5481.0	[2]
R19	$IC_6 + CH_3 = IC_6\text{-}5 + CH_4$	4.530E-01	3.650	7154.0	[2]
R20	$IC_6 + OH = IC_6\text{-}1 + H_2O$	1.056E+10	0.970	1590.0	[3]
R21	$IC_6 + OH = IC_6\text{-}2 + H_2O$	5.730E+10	0.510	63.0	[3]
R22	$IC_6 + OH = IC_6\text{-}3 + H_2O$	4.680E+07	1.610	-35.0	[3]
R23	$IC_6 + OH = IC_6\text{-}4 + H_2O$	4.680E+07	1.610	-35.0	[3]
R24	$IC_6 + OH = IC_6\text{-}5 + H_2O$	5.280E+09	0.970	1590.0	[3]
R25	$I3C_6 + H = I3C_6\text{-}1 + H_2$	1.170E+08	1.935	7650.0	[1]
R26	$I3C_6 + H = I3C_6\text{-}2 + H_2$	1.950E+08	1.840	5266.0	[1]
R27	$I3C_6 + H = I3C_6\text{-}3 + H_2$	5.700E+07	1.849	3080.0	[1]
R28	$I3C_6 + H = I3C_6\text{-}4 + H_2$	5.200E+07	1.943	7898.0	[1]
R29	$I3C_6 + CH_3 = I3C_6\text{-}1 + CH_4$	9.060E-01	3.650	7154.0	[2]
R30	$I3C_6 + CH_3 = I3C_6\text{-}2 + CH_4$	3.020E+00	3.460	5481.0	[2]

R31	$I3C_6 + CH_3 = I3C_6\text{-}3 + CH_4$	3.600E+00	3.460	4600.0	[4]
R32	$I3C_6 + CH_3 = I3C_6\text{-}4 + CH_4$	1.800E+00	3.650	7150.0	[4]
R33	$I3C_6 + OH = I3C_6\text{-}1 + H_2O$	1.056E+10	0.970	1590.0	[3]
R34	$I3C_6 + OH = I3C_6\text{-}2 + H_2O$	9.360E+07	1.610	-35.0	[3]
R35	$I3C_6 + OH = I3C_6\text{-}3 + H_2O$	5.730E+10	0.510	63.0	[3]
R36	$I3C_6 + OH = I3C_6\text{-}4 + H_2O$	5.280E+09	0.970	1590.0	[3]
R37	$XC_6 + H = XC_6\text{-}1 + H_2$	2.080E+08	1.943	7898.0	[1]
R38	$XC_6 + H = XC_6\text{-}2 + H_2$	1.425E+08	1.849	3080.0	[1]
R39	$XC_6 + CH_3 = XC_6\text{-}1 + CH_4$	7.200E+00	3.650	7150.0	[4]
R40	$XC_6 + CH_3 = XC_6\text{-}2 + CH_4$	9.000E+00	3.460	4600.0	[4]
R41	$XC_6 + OH = XC_6\text{-}1 + H_2O$	2.112E+10	0.970	1950.0	[3]
R42	$XC_6 + OH = XC_6\text{-}2 + H_2O$	1.146E+11	0.510	63.0	[3]

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