Supporting Information for

Growth Mechanism of SiC CVD – Adsorption and Surface Reactions of Active Si Species

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Table S1 Gibbs free energies of reaction (ΔG°_R) in kJ/mol at the temperature range of 298 – 2500 K.

$\Delta G^\circ_R = a_1T^4 + a_2T^3 + a_3T^2 + a_4T + a_5$ for temperature (T) = 298 – 2500 K.

		a_1	a_2	a_3	a_4	a_5
R1	SiH(g) + CH_3(ads) → SiH_2-CH_2(ads)	-2.87E-13	2.95E-09	-1.42E-05	1.54E-01	-1.61E+02
R2	SiH_2(g) + CH_3(ads) → SiH_3-CH_2(ads)	-1.37E-13	2.03E-09	-1.31E-05	1.79E-01	-2.09E+02
R3	SiCl(g) + CH_3(ads) → SiHCl-CH_2(ads)	-4.63E-13	4.20E-09	-1.76E-05	1.67E-01	-1.27E+02
R4	SiHCl(g) + CH_3(ads) → SiH_2Cl-CH_2(ads)	-3.29E-13	3.35E-09	-1.65E-05	1.93E-01	-1.89E+02
R5	$SiCl_2$(g) + CH_3(ads) → $SiHCl_2$-CH_2(ads)	-5.67E-13	5.03E-09	-2.10E-05	1.93E-01	-1.36E+02
R6	SiH(g) + CH_2(ads) → SiH-CH_2(ads)	5.36E-13	-2.93E-09	1.84E-06	1.86E-01	-3.28E+02
R7	SiH_2(g) + CH_2(ads) → SiH_2-CH_2(ads)	3.17E-13	-1.36E-09	-3.24E-06	1.79E-01	-2.54E+02
R8	SiCl(g) + CH_2(ads) → SiCl-CH_2(ads)	2.12E-13	-7.33E-10	-3.66E-06	1.93E-01	-3.10E+02
R9	SiHCl(g) + CH_2(ads) → SiHCl-CH_2(ads)	2.58E-13	-9.36E-10	-4.42E-06	1.94E-01	-2.31E+02
R10	$SiCl_2$(g) + CH_2(ads) → $SiCl_2$-CH_2(ads)	-5.17E-14	1.23E-09	-1.01E-05	1.82E-01	-1.85E+02
R11	SiH(g) + C_2H_4(ads) → SiH-$(CH_2)_2$(ads)	-3.25E-13	2.92E-09	-1.28E-05	1.60E-01	-2.80E+02
R12	SiH_2(g) + C_2H_4(ads) → SiH_2-$(CH_2)_2$(ads)	-2.19E-13	2.35E-09	-1.28E-05	1.80E-01	-3.33E+02
R13	SiCl(g) + C_2H_4(ads) → SiCl-$(CH_2)_2$(ads)	-6.34E-13	5.07E-09	-1.83E-05	1.72E-01	-2.47E+02
R14	SiHCl(g) + C_2H_4(ads) → SiHCl-$(CH_2)_2$(ads)	-5.08E-13	4.35E-09	-1.79E-05	1.94E-01	-3.15E+02
R15	$SiCl_2$(g) + C_2H_4(ads) → $SiCl_2$-$(CH_2)_2$(ads)	-7.43E-13	5.97E-09	-2.21E-05	1.98E-01	-2.75E+02
R17	C_2H_4(ads) + H(g) → CH_2(ads) + CH_3(ads)	-1.55E-13	7.55E-10	-1.21E-06	7.50E-02	-1.38E+02
R18	SiH-CH_2(ads) + CH_3(ads) → SiH_2-$(CH_2)_2$(ads)	3.94E-13	-2.44E-09	5.02E-06	3.13E-02	-2.23E+02
R19	SiH_2-CH_2(ads) + CH_3(ads) → SiH_2-$(CH_2)_2$(ads) +	-3.20E-13	2.56E-09	-7.37E-06	-6.61E-02	5.72E+01

	H(g)					
R20	$SiCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads)$	3.17E-13	-1.88E-09	3.42E-06	2.25E-02	-1.86E+02
R21	$SiHCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads) + H(g)$	-4.83E-13	3.65E-09	-1.01E-05	-6.65E-02	4.76E+01
R22	$SiCl_2\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiCl_2\text{-}(CH_2)_2(ads) + H(g)$	-5.09E-13	3.82E-09	-1.05E-05	-6.73E-02	4.43E+01
R23	$SiH_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + H_2(g)$	-8.77E-13	5.67E-09	-1.02E-05	-9.83E-02	-2.98E+01
R24	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + HCl(g)$	1.69E-13	-1.51E-09	7.59E-06	-1.26E-01	6.02E+01
R25	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + H_2(g)$	-8.65E-13	5.58E-09	-9.89E-06	-8.92E-02	-3.91E+01
R26	$SiCl_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + HCl(g)$	3.23E-13	-2.60E-09	1.05E-05	-1.22E-01	3.80E+01
R27	$SiH\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + H_2(g)$	-3.24E-13	1.42E-09	1.89E-06	-1.56E-02	-5.99E+01
R28	$SiCl\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + HCl(g)$	7.10E-13	-5.66E-09	1.94E-05	-5.25E-02	3.94E+01
R29	$SiH(g) + H(ads) \rightarrow SiH_2(ads)$	-3.13E-13	2.98E-09	-1.36E-05	1.56E-01	-1.98E+02
R30	$SiH_2(g) + H(ads) \rightarrow SiH_3(ads)$	-1.34E-13	1.91E-09	-1.23E-05	1.77E-01	-2.43E+02
R31	$SiCl(g) + H(ads) \rightarrow SiHCl(ads)$	-5.63E-13	4.71E-09	-1.81E-05	1.73E-01	-1.51E+02
R32	$SiHCl(g) + H(ads) \rightarrow SiH_2Cl(ads)$	-3.38E-13	3.29E-09	-1.57E-05	1.98E-01	-2.10E+02
R33	$SiCl_2(g) + H(ads) \rightarrow SiHCl_2(ads)$	-5.34E-13	4.68E-09	-1.94E-05	2.06E-01	-1.55E+02
R34	$SiH(g) + *(ads) \rightarrow SiH(ads)$	-7.35E-14	1.18E-09	-8.24E-06	1.69E-01	-3.45E+02
R35	$SiH_2(g) + *(ads) \rightarrow SiH_2(ads)$	-1.57E-13	1.90E-09	-1.15E-05	1.79E-01	-3.06E+02
R36	$SiCl(g) + *(ads) \rightarrow SiCl(ads)$	-3.19E-13	2.83E-09	-1.23E-05	1.83E-01	-3.39E+02
R37	$SiHCl(g) + *(ads) \rightarrow SiHCl(ads)$	-2.87E-13	2.79E-09	-1.37E-05	1.98E-01	-2.70E+02
R38	$SiCl_2(g) + *(ads) \rightarrow$	-4.28E-13	3.77E-09	-1.62E-05	2.03E-01	-2.14E+02

	$SiCl_2$(ads)					
R40	^{3}Si(g) + CH_3(ads) → SiH-CH_2(ads)	-2.19E-13	2.22E-09	-9.63E-06	1.43E-01	-2.21E+02
R41	SiF(g) + CH_3(ads) → SiHF-CH_2(ads)	-4.91E-13	4.40E-09	-1.81E-05	1.65E-01	-1.30E+02
R42	SiHF(g) + CH_3(ads) → SiH_2F-CH_2(ads)	-3.15E-13	3.26E-09	-1.63E-05	1.90E-01	-1.96E+02
R43	SiF_2(g) + CH_3(ads) → $SiHF_2$-CH_2(ads)	-5.03E-13	4.60E-09	-1.99E-05	1.89E-01	-1.41E+02
R44	SiBr(g) + CH_3(ads) → SiHBr-CH_2(ads)	-5.81E-13	5.02E-09	-1.97E-05	1.60E-01	-1.22E+02
R45	SiHBr(g) + CH_3(ads) → SiH_2Br-CH_2(ads)	-3.78E-13	3.69E-09	-1.74E-05	1.91E-01	-1.83E+02
R46	$SiBr_2$(g) + CH_3(ads) → SiHBr_2-CH_2(ads)	-5.41E-13	4.85E-09	-2.05E-05	1.94E-01	-1.32E+02
R47	^{3}Si(g) + CH_2(ads) → Si-CH_2(ads)	4.86E-13	-3.00E-09	5.37E-06	1.45E-01	-3.25E+02
R48	SiF(g) + CH_2(ads) → SiF-CH_2(ads)	1.93E-13	-6.01E-10	-4.02E-06	1.90E-01	-3.21E+02
R49	SiHF(g) + CH_2(ads) → SiHF-CH_2(ads)	2.03E-13	-5.51E-10	-5.41E-06	1.92E-01	-2.30E+02
R50	SiF_2(g) + CH_2(ads) → SiF_2-CH_2(ads)	3.17E-14	6.66E-10	-8.71E-06	1.89E-01	-1.67E+02
R51	SiBr(g) + CH_2(ads) → SiBr-CH_2(ads)	1.38E-13	-2.18E-10	-5.01E-06	1.92E-01	-3.07E+02
R52	SiHBr(g) + CH_2(ads) → SiHBr-CH_2(ads)	1.53E-13	-2.05E-10	-6.31E-06	1.87E-01	-2.28E+02
R53	$SiBr_2$(g) + CH_2(ads) → $SiBr_2$-CH_2(ads)	3.83E-14	6.19E-10	-8.57E-06	1.90E-01	-1.91E+02
R54	^{3}Si(g) + H(ads) → SiH(ads)	-3.74E-13	3.06E-09	-1.08E-05	1.28E-01	-2.23E+02
R55	SiF(g) + H(ads) → SiHF(ads)	-5.59E-13	4.70E-09	-1.82E-05	1.65E-01	-1.63E+02
R56	SiHF(g) + H(ads) → SiH_2F(ads)	-2.88E-13	2.93E-09	-1.48E-05	1.95E-01	-2.29E+02
R57	SiF_2(g) + H(ads) → $SiHF_2$(ads)	-4.21E-13	3.89E-09	-1.74E-05	2.00E-01	-1.78E+02
R58	SiBr(g) + H(ads) → SiHBr(ads)	-5.95E-13	4.93E-09	-1.86E-05	1.73E-01	-1.49E+02
R59	SiHBr(g) + H(ads) → SiH_2Br(ads)	-3.01E-13	3.02E-09	-1.50E-05	2.01E-01	-2.07E+02
R60	$SiBr_2$(g) + H(ads) → SiHBr_2(ads)	-6.27E-13	5.30E-09	-2.10E-05	2.05E-01	-1.43E+02

R61	^{3}Si(g) + *(ads) → Si(ads)	-7.90E-14	7.76E-10	-3.78E-06	1.35E-01	-3.54E+02
R62	SiF(g) + *(ads) → SiF(ads)	-2.90E-13	2.63E-09	-1.18E-05	1.82E-01	-3.58E+02
R63	SiHF(g) + *(ads) → SiHF(ads)	-3.09E-13	2.95E-09	-1.42E-05	1.90E-01	-2.78E+02
R64	SiF_2(g) + *(ads) → SiF_2(ads)	-4.33E-13	3.79E-09	-1.64E-05	1.94E-01	-2.17E+02
R65	SiBr(g) + *(ads) → SiBr(ads)	-2.20E-13	2.13E-09	-1.05E-05	1.88E-01	-3.37E+02
R66	SiHBr(g) + *(ads) → SiHBr(ads)	-3.02E-13	2.89E-09	-1.40E-05	1.98E-01	-2.71E+02
R67	$SiBr_2$(g) + *(ads) → $SiBr_2$(ads)	-4.78E-13	4.10E-09	-1.70E-05	2.05E-01	-2.12E+02

Table S2 Gibbs free energies of activation in kJ/mol at the temperature range of 298 – 2500 K.

$\Delta G^{\ddagger} = a_1T^4 + a_2T^3 + a_3T^2 + a_4T + a_5$ for temperature (T) = 298 – 2500 K.

		a_1	a_2	a_3	a_4	a_5
R1	SiH(g) + CH_3(ads) → SiH_2-CH_2(ads)	-4.57E-13	3.78E-09	-1.32E-05	1.46E-01	7.82E+01
R2	SiH_2(g) + CH_3(ads) → SiH_3-CH_2(ads)	-3.76E-13	3.31E-09	-1.32E-05	1.65E-01	8.32E+01
R3	SiCl(g) + CH_3(ads) → SiHCl-CH_2(ads)	-7.22E-13	5.60E-09	-1.79E-05	1.54E-01	1.05E+02
R4	SiHCl(g) + CH_3(ads) → SiH_2Cl-CH_2(ads)	-5.83E-13	4.75E-09	-1.70E-05	1.80E-01	1.20E+02
R5	$SiCl_2$(g) + CH_3(ads) → $SiHCl_2$-CH_2(ads)	-7.00E-13	5.60E-09	-1.94E-05	1.83E-01	1.89E+02
R11	SiH(g) + C_2H_4(ads) → SiH-$(CH_2)_2$(ads)	-6.81E-13	4.99E-09	-1.48E-05	1.44E-01	1.38E+02
R12	SiH_2(g) + C_2H_4(ads) → SiH_2-$(CH_2)_2$(ads)	-8.40E-13	6.23E-09	-1.94E-05	1.57E-01	2.04E+02
R13	SiCl(g) + C_2H_4(ads) → SiCl-$(CH_2)_2$(ads)	-9.03E-13	6.49E-09	-1.85E-05	1.45E-01	1.49E+02
R14	SiHCl(g) + C_2H_4(ads) → SiHCl-$(CH_2)_2$(ads)	-9.87E-13	7.22E-09	-2.18E-05	1.73E-01	2.34E+02
R15	$SiCl_2$(g) + C_2H_4(ads) → $SiCl_2$-$(CH_2)_2$(ads)	-1.20E-12	8.65E-09	-2.53E-05	1.71E-01	2.78E+02

R18	$SiH\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiH_2\text{-}(CH_2)_2(ads)$	2.85E-13	-2.08E-09	7.37E-06	2.31E-02	9.17E+01
R19	$SiH_2\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiH_2\text{-}(CH_2)_2(ads) + H(g)$	1.72E-13	-1.03E-09	3.51E-06	3.51E-02	1.73E+02
R20	$SiCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads)$	1.75E-13	-1.30E-09	5.24E-06	1.27E-02	1.41E+02
R21	$SiHCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads) + H(g)$	1.05E-13	-5.95E-10	2.48E-06	3.52E-02	1.63E+02
R22	$SiCl_2\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiCl_2\text{-}(CH_2)_2(ads) + H(g)$	9.10E-15	2.02E-10	-2.47E-07	2.16E-02	1.87E+02
R23	$SiH_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + H_2(g)$	1.06E-13	-4.55E-10	1.42E-06	8.37E-03	2.90E+02
R24	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + HCl(g)$	2.71E-13	-2.01E-09	7.14E-06	1.33E-02	2.29E+02
R25	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + H_2(g)$	1.16E-13	-6.45E-10	2.42E-06	9.80E-03	2.65E+02
R26	$SiCl_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + HCl(g)$	5.25E-13	-3.65E-09	1.09E-05	1.45E-02	2.40E+02
R27	$SiH\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + H_2(g)$	1.95E-13	-1.46E-09	5.04E-06	8.58E-02	9.45E+00
R28	$SiCl\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + HCl(g)$	3.24E-13	-2.40E-09	7.67E-06	8.36E-02	8.60E+01
R29	$SiH(g) + H(ads) \rightarrow SiH_2(ads)$	-3.92E-13	3.16E-09	-1.09E-05	1.44E-01	4.48E+01
R30	$SiH_2(g) + H(ads) \rightarrow SiH_3(ads)$	-3.15E-13	2.75E-09	-1.11E-05	1.70E-01	5.73E+01
R31	$SiCl(g) + H(ads) \rightarrow SiHCl(ads)$	-6.32E-13	4.81E-09	-1.51E-05	1.54E-01	7.82E+01
R32	$SiHCl(g) + H(ads) \rightarrow SiH_2Cl(ads)$	-6.07E-13	4.72E-09	-1.60E-05	1.82E-01	1.15E+02
R33	$SiCl_2(g) + H(ads) \rightarrow SiHCl_2(ads)$	-7.37E-13	5.66E-09	-1.86E-05	1.88E-01	1.92E+02

Table S3 Sticking coefficients, $S = AT^n exp(-E/RT)$, at the temperature range of 298 – 2500 K. The energy (E) is in the unit of kJ/mol.

		S	298 – 2500 K		
		(1600 °C)	ln (A)	n	E
R1	$SiH(g) + CH_3(ads) \rightarrow SiH_2\text{-}CH_2(ads)$	3.02E-04	-22.215	2.524	76.516
R2	$SiH_2(g) + CH_3(ads) \rightarrow SiH_3\text{-}CH_2(ads)$	2.60E-05	-25.921	2.727	80.711
R3	$SiCl(g) + CH_3(ads) \rightarrow SiHCl\text{-}CH_2(ads)$	4.33E-05	-23.879	2.716	103.288
R4	$SiHCl(g) + CH_3(ads) \rightarrow SiH_2Cl\text{-}CH_2(ads)$	7.03E-07	-28.371	2.889	117.891
R5	$SiCl_2(g) + CH_3(ads) \rightarrow SiHCl_2\text{-}CH_2(ads)$	8.15E-09	-29.411	3.018	186.254
R11	$SiH(g) + C_2H_4(ads) \rightarrow SiH\text{-}(CH_2)_2(ads)$	9.48E-06	-20.860	2.397	136.556
R12	$SiH_2(g) + C_2H_4(ads) \rightarrow SiH_2\text{-}(CH_2)_2(ads)$	5.31E-08	-24.845	2.795	202.007
R13	$SiCl(g) + C_2H_4(ads) \rightarrow SiCl\text{-}(CH_2)_2(ads)$	6.61E-06	-21.531	2.533	147.736
R14	$SiHCl(g) + C_2H_4(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads)$	1.68E-09	-27.043	2.883	231.808
R15	$SiCl_2(g) + C_2H_4(ads) \rightarrow SiCl_2\text{-}(CH_2)_2(ads)$	1.98E-10	-27.388	3.019	275.674
R29	$SiH(g) + H(ads) \rightarrow SiH_2(ads)$	2.62E-03	-20.912	2.355	43.270
R30	$SiH_2(g) + H(ads) \rightarrow SiH_3(ads)$	6.35E-05	-25.508	2.572	55.036
R31	$SiCl(g) + H(ads) \rightarrow SiHCl(ads)$	1.88E-04	-22.666	2.523	76.678
R32	$SiHCl(g) + H(ads) \rightarrow SiH_2Cl(ads)$	7.69E-07	-27.618	2.754	112.348
R33	$SiCl_2(g) + H(ads) \rightarrow SiHCl_2(ads)$	3.67E-09	-28.940	2.881	189.888

Table S4 Rate constants in forward and reverse directions. A and E are in the units of molecules per site per second and kJ/mol.

		Forward rate constants	Reverse rate constants

		ln (A)	n	E	ln (A)	n	E
R18	$SiH\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiH_2\text{-}(CH_2)_2(ads)$	25.088	0.334	93.129	28.915	0.381	316.595
R19	$SiH_2\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiH_2\text{-}(CH_2)_2(ads) + H(g)$	21.913	0.629	173.923	3.526	0.450	116.164
R20	$SiCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads)$	25.760	0.442	141.871	28.983	0.405	328.009
R21	$SiHCl\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiHCl\text{-}(CH_2)_2(ads) + H(g)$	21.767	0.663	163.960	3.809	0.382	115.888
R22	$SiCl_2\text{-}CH_2(ads) + CH_3(ads) \rightarrow SiCl_2\text{-}(CH_2)_2(ads) + H(g)$	22.261	0.859	187.453	6.906	0.240	145.684
R23	$SiH_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + H_2(g)$	24.102	0.799	290.502	-3.375	1.370	316.249
R24	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiH\text{-}(CH_2)_3(ads) + HCl(g)$	26.089	0.362	230.300	-6.274	1.372	167.938
R25	$SiHCl\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + H_2(g)$	24.630	0.688	266.089	-2.919	1.274	301.090
R26	$SiCl_2\text{-}(CH_2)_2(ads) + CH_3(ads) \rightarrow SiCl\text{-}(CH_2)_3(ads) + HCl(g)$	25.932	0.311	241.019	-7.590	1.435	201.034
R27	$SiH\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + H_2(g)$	6.449	0.603	10.898	-3.942	1.654	66.495
R28	$SiCl\text{-}(CH_2)_3(ads) + H(g) \rightarrow Si^*\text{-}(CH_2)_3(ads) + HCl(g)$	6.141	0.492	87.315	-8.998	1.959	45.603
R29	$SiH(g) + H(ads) \rightarrow SiH_2(ads)$	-10.563	1.884	43.884	29.320	0.393	244.838
R30	$SiH_2(g) + H(ads) \rightarrow SiH_3(ads)$	-15.192	2.103	55.638	28.581	0.428	302.576
R31	$SiCl(g) + H(ads) \rightarrow SiHCl(ads)$	-12.736	2.056	77.259	30.230	0.372	230.536
R32	$SiHCl(g) + H(ads) \rightarrow SiH_2Cl(ads)$	-17.679	2.285	112.951	29.360	0.486	326.841
R33	$SiCl_2(g) + H(ads) \rightarrow SiHCl_2(ads)$	-19.224	2.413	190.480	29.782	0.449	349.358

Table S4 Molecular Coordinates in Z-matrix form

CH_3(ads)

Si

Si	1	B1				
Si	1	B2	2	A1		
Si	2	B3	1	A2	3	D1
Si	2	B4	1	A3	3	D2
Si	5	B5	2	A4	1	D3
Si	3	B6	1	A5	6	D4
Si	2	B7	1	A6	3	D5
Si	2	B8	1	A7	3	D6
Si	7	B9	3	A8	1	D7
Si	9	B10	2	A9	1	D8
Si	3	B11	1	A10	6	D9
C	6	B12	5	A11	2	D10
C	1	B13	3	A12	12	D11
C	2	B14	1	A13	14	D12
C	12	B15	3	A14	1	D13
C	11	B16	9	A15	2	D14
C	10	B17	7	A16	3	D15
C	7	B18	3	A17	1	D16
C	12	B19	3	A18	1	D17
C	7	B20	3	A19	1	D18
C	9	B21	2	A20	1	D19
H	1	B22	14	A21	3	D20
H	2	B23	1	A22	14	D21
H	3	B24	1	A23	14	D22
H	5	B25	2	A24	1	D23
H	16	B26	12	A25	3	D24
H	6	B27	5	A26	2	D25
H	17	B28	11	A27	9	D26
H	18	B29	10	A28	7	D27
H	19	B30	7	A29	3	D28
H	20	B31	12	A30	3	D29
H	21	B32	7	A31	3	D30
H	22	B33	9	A32	2	D31
C	4	B34	2	A33	1	D32
C	3	B35	1	A34	14	D33
Si	20	B36	12	A35	3	D34
Si	19	B37	7	A36	3	D35
C	38	B38	19	A37	7	D36
Si	36	B39	3	A38	1	D37
H	39	B40	38	A39	19	D38
H	39	B41	38	A40	19	D39
H	40	B42	36	A41	3	D40
H	40	B43	36	A42	3	D41
H	38	B44	19	A43	7	D42
H	7	B45	3	A44	1	D43
H	36	B46	3	A45	1	D44
H	14	B47	1	A46	3	D45
H	13	B48	6	A47	5	D46
H	11	B49	9	A48	2	D47
C	1	B50	14	A49	3	D48
C	2	B51	1	A50	14	D49
C	3	B52	1	A51	14	D50

Si	53	B53	3	A52	1	D51
H	5	B54	2	A53	1	D52
H	2	B55	1	A54	14	D53
H	22	B56	9	A55	2	D54
H	17	B57	11	A56	9	D55
H	21	B58	7	A57	3	D56
H	18	B59	10	A58	7	D57
H	6	B60	5	A59	2	D58
H	1	B61	14	A60	3	D59
Si	15	B62	2	A61	1	D60
Si	35	B63	4	A62	2	D61
C	37	B64	20	A63	12	D62
C	8	B65	2	A64	1	D63
H	63	B66	15	A65	2	D64
H	64	B67	35	A66	4	D65
H	64	B68	35	A67	4	D66
H	63	B69	15	A68	2	D67
C	64	B70	35	A69	4	D68
H	65	B71	37	A70	20	D69
H	65	B72	37	A71	20	D70
H	66	B73	8	A72	2	D71
H	66	B74	8	A73	2	D72
Si	66	B75	8	A74	2	D73
H	76	B76	66	A75	8	D74
H	71	B77	64	A76	35	D75
C	4	B78	2	A77	1	D76
H	79	B79	4	A78	2	D77
H	79	B80	4	A79	2	D78
H	54	B81	53	A80	3	D79
H	79	B82	4	A81	2	D80

B1	6.23695371
B2	3.12466288
B3	3.12492341
B4	3.123748
B5	3.11360127
B6	3.15242921
B7	3.14264496
B8	3.15080112
B9	3.14880025
B10	3.15449541
B11	3.13241433
B12	1.90864347
B13	1.90534656
B14	1.90920433
B15	1.9106695
B16	1.90549562
B17	1.90663972
B18	1.90945671
B19	1.90657797
B20	1.90315855

B21	1.89975592
B22	1.48965657
B23	1.48886898
B24	1.49044657
B25	1.48935948
B26	1.10471968
B27	1.48937652
B28	1.10077657
B29	1.10075451
B30	1.10294289
B31	1.10455576
B32	1.10050522
B33	1.10101112
B34	1.93631945
B35	1.91121155
B36	1.91170394
B37	1.90935512
B38	1.9024026
B39	1.90653681
B40	1.09904874
B41	1.10059757
B42	1.49062268
B43	1.48861562
B44	1.4920251
B45	1.49201658
B46	1.10126326
B47	1.10123542
B48	1.10075061
B49	1.4915356
B50	1.91055093
B51	1.90942482
B52	1.91823329
B53	1.91381942
B54	1.49049547
B55	1.49118893
B56	1.09913163
B57	1.09906535
B58	1.09941758
B59	1.09908069
B60	1.49048433
B61	1.49078801
B62	1.9113737
B63	1.91175397
B64	1.90737225
B65	1.90659095
B66	1.48848057
B67	1.49035091
B68	1.48845438
B69	1.49046071
B70	1.90968814
B71	1.10076914
B72	1.09877357

B73	1.10083295
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B75	1.90454905
B76	1.49154792
B77	1.1008333
B78	1.90031252
B79	1.09563977
B80	1.09538386
B81	1.49083547
B82	1.09547668
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A8	90.22948376
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A10	90.30442162
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A12	35.0643815
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A21	110.2257498
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A23	88.98135511
A24	90.33554663
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A28	108.2908169
A29	108.3601459
A30	107.4669778
A31	109.1951214
A32	108.4688791
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A34	146.6052331
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A36	111.6411974
A37	108.3644683
A38	110.8960034
A39	110.6814595
A40	109.1472346
A41	110.4476997
A42	110.3536357

A43	110.500461
A44	121.8178193
A45	107.6084554
A46	108.0689729
A47	108.1054229
A48	145.4595358
A49	108.5718294
A50	36.11312732
A51	89.87346829
A52	110.2732459
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A54	145.6689508
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A67	110.6814488
A68	110.0220489
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A70	108.0157387
A71	110.0771132
A72	108.0039563
A73	110.0758336
A74	111.7218846
A75	111.5496859
A76	107.9638165
A77	90.25632532
A78	111.05412
A79	111.5952142
A80	109.6822087
A81	111.0352965
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D4	109.296205
D5	-54.35051215
D6	-109.1082648
D7	-54.37737111
D8	-69.94345952
D9	54.33324609
D10	142.1323596
D11	-87.799067
D12	1.74596961
D13	-13.6888881

D14	-109.5536475
D15	163.1627898
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D17	-164.6299641
D18	-43.73605895
D19	142.5899682
D20	56.55185004
D21	112.1358392
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D28	178.887737
D29	-143.965859
D30	-138.8950368
D31	-176.6807499
D32	-144.1122691
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D34	-26.80460128
D35	-61.90128408
D36	-178.533856
D37	179.3429321
D38	174.7710776
D39	57.51704687
D40	-177.6577624
D41	-59.53794311
D42	-56.317336
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D44	61.39967194
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D46	117.4224534
D47	-104.0508683
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D50	-123.6994095
D51	-27.76330527
D52	163.5445222
D53	-126.5386452
D54	66.65338846
D55	123.0870013
D56	103.9181161
D57	-55.97921494
D58	149.3345801
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D60	149.5368392
D61	-60.67368947
D62	-178.2588684
D63	165.2435101
D64	-59.02971388
D65	-178.6207151

D66	-60.52071304
D67	59.08141777
D68	60.44803912
D69	59.61517649
D70	175.7985336
D71	147.145078
D72	31.01377836
D73	-92.94325203
D74	176.4491745
D75	-179.691156
D76	89.78410697
D77	-30.87090716
D78	89.34272402
D79	-60.9034913
D80	-150.4694348

CH_2(ads)

Si						
Si	1	B1				
Si	1	B2	2	A1		
Si	2	B3	1	A2	3	D1
Si	2	B4	1	A3	3	D2
Si	5	B5	2	A4	1	D3
Si	3	B6	1	A5	6	D4
Si	2	B7	1	A6	3	D5
Si	8	B8	2	A7	1	D6
Si	7	B9	3	A8	1	D7
Si	9	B10	8	A9	2	D8
Si	3	B11	1	A10	6	D9
C	6	B12	5	A11	2	D10
C	1	B13	3	A12	4	D11
C	2	B14	1	A13	14	D12
C	12	B15	3	A14	1	D13
C	11	B16	9	A15	8	D14
C	10	B17	7	A16	3	D15
C	7	B18	3	A17	1	D16
C	12	B19	3	A18	1	D17
C	7	B20	3	A19	1	D18
C	9	B21	8	A20	2	D19
H	1	B22	14	A21	3	D20
H	2	B23	1	A22	14	D21
H	3	B24	1	A23	14	D22
H	5	B25	2	A24	1	D23
H	16	B26	12	A25	3	D24
H	6	B27	5	A26	2	D25
H	17	B28	11	A27	9	D26
H	18	B29	10	A28	7	D27
H	19	B30	7	A29	3	D28
H	20	B31	12	A30	3	D29
H	21	B32	7	A31	3	D30

H	22	B33	9	A32	8	D31
C	4	B34	2	A33	1	D32
C	3	B35	1	A34	14	D33
Si	20	B36	12	A35	3	D34
Si	19	B37	7	A36	3	D35
C	38	B38	19	A37	7	D36
Si	36	B39	3	A38	1	D37
H	39	B40	38	A39	19	D38
H	39	B41	38	A40	19	D39
H	40	B42	36	A41	3	D40
H	40	B43	36	A42	3	D41
H	38	B44	19	A43	7	D42
H	7	B45	3	A44	1	D43
H	36	B46	3	A45	1	D44
H	14	B47	1	A46	3	D45
H	13	B48	6	A47	5	D46
H	11	B49	9	A48	8	D47
C	1	B50	14	A49	3	D48
C	2	B51	1	A50	14	D49
C	3	B52	1	A51	14	D50
Si	53	B53	3	A52	1	D51
H	5	B54	2	A53	1	D52
H	2	B55	1	A54	14	D53
H	22	B56	9	A55	8	D54
H	17	B57	11	A56	9	D55
H	21	B58	7	A57	3	D56
H	18	B59	10	A58	7	D57
H	6	B60	5	A59	2	D58
H	1	B61	14	A60	3	D59
Si	15	B62	2	A61	1	D60
Si	35	B63	4	A62	2	D61
C	37	B64	20	A63	12	D62
C	8	B65	2	A64	1	D63
H	63	B66	15	A65	2	D64
H	64	B67	35	A66	4	D65
H	64	B68	35	A67	4	D66
H	63	B69	15	A68	2	D67
C	64	B70	35	A69	4	D68
H	65	B71	37	A70	20	D69
H	65	B72	37	A71	20	D70
H	66	B73	8	A72	2	D71
H	66	B74	8	A73	2	D72
Si	66	B75	8	A74	2	D73
H	76	B76	66	A75	8	D74
H	71	B77	64	A76	35	D75
C	4	B78	2	A77	1	D76
H	79	B79	4	A78	2	D77
H	79	B80	4	A79	2	D78
H	54	B81	53	A80	3	D79

B1	6.22824254
B2	3.12490123
B3	3.11769344
B4	3.12555538
B5	3.11415772
B6	3.15353153
B7	3.15295864
B8	3.15522111
B9	3.14998184
B10	3.15472409
B11	3.13836119
B12	1.9085515
B13	1.90510444
B14	1.90982966
B15	1.91019619
B16	1.90539133
B17	1.90657123
B18	1.9096806
B19	1.90777412
B20	1.90354238
B21	1.89963673
B22	1.4897187
B23	1.4885418
B24	1.49023158
B25	1.48931876
B26	1.10471142
B27	1.48940192
B28	1.10076809
B29	1.1007567
B30	1.10294982
B31	1.10460165
B32	1.10052632
B33	1.10098491
B34	1.93481672
B35	1.91026996
B36	1.9128069
B37	1.91023303
B38	1.90285581
B39	1.90681209
B40	1.09914228
B41	1.10058363
B42	1.49113467
B43	1.48805051
B44	1.49201457
B45	1.49200453
B46	1.10124273
B47	1.10123652
B48	1.10075443
B49	1.49153045
B50	1.91061018
B51	1.91013231
B52	1.91833739

B53	1.9136359
B54	1.49042434
B55	1.49149626
B56	1.09925739
B57	1.09906132
B58	1.09942028
B59	1.09907853
B60	1.49046218
B61	1.49077471
B62	1.91107839
B63	1.91121531
B64	1.90727209
B65	1.90624271
B66	1.48849438
B67	1.49022568
B68	1.48888723
B69	1.49049944
B70	1.9084041
B71	1.1007758
B72	1.09885603
B73	1.10080256
B74	1.09889069
B75	1.90439814
B76	1.49151902
B77	1.10080647
B78	1.86766338
B79	1.0898424
B80	1.08975628
B81	1.49144874
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A3	60.11405267
A4	119.8942606
A5	60.64600037
A6	90.95805095
A7	60.07339087
A8	90.20663027
A9	179.4864505
A10	90.28431963
A11	35.35149239
A12	35.07870747
A13	91.14325574
A14	121.3768814
A15	34.12974338
A16	146.5961692
A17	72.53361681
A18	121.3653066
A19	122.8975723
A20	33.89266089
A21	110.2349437
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A23	88.96275535

A24	90.1387376
A25	107.3164398
A26	88.99797365
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A28	108.2985062
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A47	108.1034335
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A50	36.45644291
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A52	110.1555727
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A68	109.9924038
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A75	111.5267518

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A77	90.23301704
A78	122.0972651
A79	122.7855673
A80	109.5382584
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D2	-179.6768661
D3	0.13656947
D4	109.3723906
D5	-54.67483828
D6	-55.34938723
D7	-54.40525896
D8	27.79525413
D9	54.52863435
D10	142.3873464
D11	-143.0649499
D12	1.03929034
D13	-14.00009144
D14	-137.5440625
D15	163.0759129
D16	-144.91426
D17	-164.6077111
D18	-43.8056561
D19	-109.9990011
D20	56.55843914
D21	111.0391832
D22	126.714826
D23	-88.90961264
D24	144.1720466
D25	-89.4873785
D26	-119.6625984
D27	60.34366479
D28	179.1075166
D29	-144.1265996
D30	-138.8425328
D31	-119.7031241
D32	-145.4905877
D33	0.86713334
D34	-27.00055431
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D50	-123.3956914
D51	-28.15953354
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D53	-127.9165842
D54	123.6303401
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D57	-55.91740806
D58	149.6135921
D59	175.4353412
D60	148.8896705
D61	-59.53976182
D62	-178.3274472
D63	165.1107586
D64	-59.02973637
D65	-178.2848989
D66	-60.20673407
D67	59.31698889
D68	60.55908158
D69	59.65566198
D70	175.8542363
D71	147.3249355
D72	31.17488684
D73	-92.61468241
D74	176.6370447
D75	-179.8071393
D76	89.04232718
D77	-73.62401135
D78	105.0392254

C_2H_4(ads)

Si						
Si	1	B1				
Si	1	B2	2	A1		
Si	3	B3	1	A2	2	D1
Si	2	B4	1	A3	3	D2
Si	5	B5	2	A4	1	D3
Si	3	B6	1	A5	6	D4
Si	2	B7	1	A6	3	D5
Si	2	B8	1	A7	3	D6
Si	1	B9	3	A8	4	D7
Si	10	B10	1	A9	3	D8
Si	7	B11	3	A10	1	D9
C	5	B12	2	A11	1	D10
C	3	B13	1	A12	6	D11
C	2	B14	1	A13	14	D12
C	12	B15	7	A14	3	D13
C	9	B16	2	A15	1	D14

C	11	B17	10	A16	1	D15
C	7	B18	3	A17	1	D16
C	12	B19	7	A18	3	D17
C	7	B20	3	A19	1	D18
C	8	B21	2	A20	1	D19
H	1	B22	14	A21	3	D20
H	2	B23	1	A22	14	D21
H	3	B24	1	A23	14	D22
H	5	B25	2	A24	1	D23
H	16	B26	12	A25	7	D24
H	6	B27	5	A26	2	D25
H	17	B28	9	A27	2	D26
H	18	B29	11	A28	10	D27
H	19	B30	7	A29	3	D28
H	20	B31	12	A30	7	D29
H	21	B32	7	A31	3	D30
H	22	B33	8	A32	2	D31
C	4	B34	3	A33	1	D32
C	3	B35	1	A34	14	D33
Si	20	B36	12	A35	7	D34
Si	19	B37	7	A36	3	D35
C	38	B38	19	A37	7	D36
Si	36	B39	3	A38	1	D37
H	39	B40	38	A39	19	D38
H	39	B41	38	A40	19	D39
H	40	B42	36	A41	3	D40
H	40	B43	36	A42	3	D41
H	38	B44	19	A43	7	D42
H	7	B45	3	A44	1	D43
H	36	B46	3	A45	1	D44
H	14	B47	3	A46	1	D45
H	13	B48	5	A47	2	D46
H	11	B49	10	A48	1	D47
C	6	B50	5	A49	2	D48
C	2	B51	1	A50	14	D49
C	12	B52	7	A51	3	D50
Si	53	B53	12	A52	7	D51
H	5	B54	2	A53	1	D52
H	2	B55	1	A54	14	D53
H	22	B56	8	A55	2	D54
H	17	B57	9	A56	2	D55
H	21	B58	7	A57	3	D56
H	18	B59	11	A58	10	D57
H	6	B60	5	A59	2	D58
H	1	B61	14	A60	3	D59
Si	15	B62	2	A61	1	D60
Si	35	B63	4	A62	3	D61
C	37	B64	20	A63	12	D62
C	8	B65	2	A64	1	D63
H	63	B66	15	A65	2	D64
H	64	B67	35	A66	4	D65
H	64	B68	35	A67	4	D66

H	63	B69	15	A68	2	D67
C	63	B70	15	A69	2	D68
H	65	B71	37	A70	20	D69
H	65	B72	37	A71	20	D70
H	66	B73	8	A72	2	D71
H	66	B74	8	A73	2	D72
Si	65	B75	37	A74	20	D73
H	76	B76	65	A75	37	D74
H	71	B77	63	A76	15	D75
C	4	B78	3	A77	1	D76
H	79	B79	4	A78	3	D77
H	79	B80	4	A79	3	D78
C	79	B81	4	A80	3	D79
H	82	B82	79	A81	4	D80
H	82	B83	79	A82	4	D81

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B6	3.12044014
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B9	3.13796728
B10	3.15294888
B11	3.14489532
B12	1.90271594
B13	1.8994673
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B15	1.91266803
B16	1.90716515
B17	1.90197548
B18	1.91993913
B19	1.91268726
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B26	1.10448565
B27	1.49059692
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B30	1.10295934
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A81	109.4176879
A82	109.9503
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