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Supplementary material

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Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories

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Supporting Information

Table S1: Unimolecular rate constants for all reaction steps involved in the reported chemical pathways (results obtained by means of RRKM theory at different pressures and temperatures, according to the computed UM06-2x/aug-cc-pVTZ energy profiles).

Table S1a: [$T = 570$ K]

P (bar)	k_{uni} (R1→P1)	k_{uni} (R2→P2)	k_{uni} (R3→P3)	k_{uni} (R4→P4)	$\log P$	$\log k_{\text{uni}}$ (R1→P1)	$\log k_{\text{uni}}$ (R2→P2)	$\log k_{\text{uni}}$ (R3→P3)	$\log k_{\text{uni}}$ (R4→P4)
1.00E+02	6.78E-06	5.33E-06	2.95E-05	6.88E-03	2	-5.17	-5.27	-4.53	-2.16
1.00E+00	6.78E-06	5.33E-06	2.95E-05	6.88E-03	0	-5.17	-5.27	-4.53	-2.16
1.00E-02	6.76E-06	5.33E-06	2.95E-05	6.88E-03	-2	-5.17	-5.27	-4.53	-2.16
1.00E-04	6.00E-06	5.29E-06	2.94E-05	6.81E-03	-4	-5.22	-5.28	-4.53	-2.17
1.00E-06	2.62E-06	4.37E-06	2.63E-05	5.39E-03	-6	-5.58	-5.36	-4.58	-2.27
1.00E-08	3.69E-07	1.63E-06	1.24E-05	1.75E-03	-8	-6.43	-5.79	-4.91	-2.76
1.00E-10	1.92E-08	2.09E-07	2.03E-06	1.81E-04	-10	-7.72	-6.68	-5.69	-3.74
1.00E-12	4.96E-10	1.10E-08	1.28E-07	7.82E-06	-12	-9.30	-7.96	-6.89	-5.11

Table S1b: [$T = 600$ K]

P (bar)	k_{uni} (R1→P1)	k_{uni} (R2→P2)	k_{uni} (R3→P3)	k_{uni} (R4→P4)	$\log P$	$\log k_{\text{uni}}$ (R1→P1)	$\log k_{\text{uni}}$ (R2→P2)	$\log k_{\text{uni}}$ (R3→P3)	$\log k_{\text{uni}}$ (R4→P4)
1.00E+02	5.48E-05	4.34E-05	2.34E-04	4.22E-02	2	-4.26	-4.36	-3.63	-1.37
1.00E+00	5.48E-05	4.34E-05	2.34E-04	4.22E-02	0	-4.26	-4.36	-3.63	-1.37
1.00E-02	5.45E-05	4.34E-05	2.34E-04	4.22E-02	-2	-4.26	-4.36	-3.63	-1.37
1.00E-04	4.60E-05	4.28E-05	2.32E-04	4.14E-02	-4	-4.34	-4.37	-3.63	-1.38
1.00E-06	1.73E-05	3.25E-05	1.94E-04	2.90E-02	-6	-4.76	-4.49	-3.71	-1.54
1.00E-08	2.07E-06	1.00E-05	7.48E-05	7.29E-03	-8	-5.68	-5.00	-4.13	-2.14
1.00E-10	9.54E-08	1.07E-06	9.68E-06	5.80E-04	-10	-7.02	-5.97	-5.01	-3.24
1.00E-12	2.30E-09	4.86E-08	5.09E-07	2.09E-05	-12	-8.64	-7.31	-6.29	-4.68

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Table S1c: [$T = 630$ K]

P (bar)	k_{uni} (R1→P1)	k_{uni} (R2→P2)	k_{uni} (R3→P3)	k_{uni} (R4→P4)	$\log P$	$\log k_{\text{uni}}$ (R1→P1)	$\log k_{\text{uni}}$ (R2→P2)	$\log k_{\text{uni}}$ (R3→P3)	$\log k_{\text{uni}}$ (R4→P4)
1.00E+02	3.64E-04	2.89E-04	1.52E-03	2.18E-01	2	-3.44	-3.54	-2.82	-0.66
1.00E+00	3.64E-04	2.89E-04	1.52E-03	2.18E-01	0	-3.44	-3.54	-2.82	-0.66
1.00E-02	3.60E-04	2.89E-04	1.52E-03	2.18E-01	-2	-3.44	-3.54	-2.82	-0.66
1.00E-04	2.87E-04	2.82E-04	1.50E-03	2.10E-01	-4	-3.54	-3.55	-2.82	-0.68
1.00E-06	9.20E-05	1.95E-04	1.15E-03	1.27E-01	-6	-4.04	-3.71	-2.94	-0.90
1.00E-08	9.46E-06	4.94E-05	3.59E-04	2.45E-02	-8	-5.02	-4.31	-3.44	-1.61
1.00E-10	3.92E-07	4.41E-06	3.71E-05	1.54E-03	-10	-6.41	-5.36	-4.43	-2.81
1.00E-12	8.83E-09	1.76E-07	1.66E-06	4.68E-05	-12	-8.05	-6.76	-5.78	-4.33

Table S1d: [$T = 660$ K]

P (bar)	k_{uni} (R1→P1)	k_{uni} (R2→P2)	k_{uni} (R3→P3)	k_{uni} (R4→P4)	$\log P$	$\log k_{\text{uni}}$ (R1→P1)	$\log k_{\text{uni}}$ (R2→P2)	$\log k_{\text{uni}}$ (R3→P3)	$\log k_{\text{uni}}$ (R4→P4)
1.00E+02	2.03E-03	1.63E-03	8.34E-03	9.74E-01	2	-2.69	-2.79	-2.08	-0.01
1.00E+00	2.03E-03	1.63E-03	8.34E-03	9.74E-01	0	-2.69	-2.79	-2.08	-0.01
1.00E-02	2.00E-03	1.63E-03	8.34E-03	9.73E-01	-2	-2.70	-2.79	-2.08	-0.01
1.00E-04	1.49E-03	1.56E-03	8.15E-03	9.12E-01	-4	-2.83	-2.81	-2.09	-0.04
1.00E-06	4.09E-04	9.60E-04	5.59E-03	4.63E-01	-6	-3.39	-3.02	-2.25	-0.33
1.00E-08	3.64E-05	2.01E-04	1.41E-03	6.84E-02	-8	-4.44	-3.70	-2.85	-1.17
1.00E-10	1.37E-06	1.52E-05	1.18E-04	3.46E-03	-10	-5.86	-4.82	-3.93	-2.46
1.00E-12	2.90E-08	5.35E-07	4.55E-06	9.08E-05	-12	-7.54	-6.27	-5.34	-4.04

Table S1e: [$T = 690$ K]

P (bar)	k_{uni} (R1→P1)	k_{uni} (R2→P2)	k_{uni} (R3→P3)	k_{uni} (R4→P4)	$\log P$	$\log k_{\text{uni}}$ (R1→P1)	$\log k_{\text{uni}}$ (R2→P2)	$\log k_{\text{uni}}$ (R3→P3)	$\log k_{\text{uni}}$ (R4→P4)
1.00E+02	9.80E-03	7.89E-03	3.95E-02	3.82E+00	2.00	-2.01	-2.10	-1.40	0.58
1.00E+00	9.80E-03	7.89E-03	3.95E-02	3.82E+00	0.00	-2.01	-2.10	-1.40	0.58
1.00E-02	9.59E-03	7.88E-03	3.95E-02	3.81E+00	-2.00	-2.02	-2.10	-1.40	0.58
1.00E-04	6.57E-03	7.41E-03	3.80E-02	3.43E+00	-4.00	-2.18	-2.13	-1.42	0.54
1.00E-06	1.55E-03	3.99E-03	2.29E-02	1.43E+00	-6.00	-2.81	-2.40	-1.64	0.16
1.00E-08	1.21E-04	6.94E-04	4.65E-03	1.63E-01	-8.00	-3.92	-3.16	-2.33	-0.79
1.00E-10	4.13E-06	4.51E-05	3.20E-04	6.80E-03	-10.00	-5.38	-4.35	-3.49	-2.17
1.00E-12	8.29E-08	1.41E-06	1.08E-05	1.56E-04	-12.00	-7.08	-5.85	-4.97	-3.81