

Supporting information

Mechanism of Formation of Chlorinated Pyrene during Combustion of Polyvinyl Chloride

**Yuichi Miyake,[†] Masahiro Tokumura,[†] Qi Wang,[†] Takashi Amagai,^{†,*} Yuichi Horii,[‡] and
Kurunthachalam Kannan^{§,||*}**

[†]Graduate School of Nutritional and Environmental Science, University of Shizuoka, Shizuoka,
Japan

[‡]Center for Environmental Science in Saitama, 914 Kamitanadare, Kazo, Saitama, Japan

[§]Wadsworth Center, New York State Department of Health, and Department of Environmental
Health Sciences, State University of New York at Albany, New York, United States

^{||}Biochemistry Department, Faculty of Science and Experimental Biochemistry Unit, King Fahd
Medical Research Center, King Abdulaziz University, Jeddah 21589, Saudi Arabia

Corresponding authors

*Phone/Fax: +81-54-264-5789 (T.A.); Email: amagai@u-shizuoka-ken.ac.jp

*Phone: 518-474-0015, Fax: 518-473-2895 (K.K.); Email:

Kurunthachalam.kannan@health.ny.gov

19 Table S1 Formation and decomposition rate constants of precursor, pyrene, and chlorinated pyrenes
 20 (the initial concentration of the precursor: 1000 nmol m⁻³).

Temperature		Formation rate constants (sec ⁻¹)					
(°C)	(1/K)	k_1	k_2	k_3	k_4	k_5	k_6
800	0.00093	0.005	3	0.5	4	0.7	0.35
900	0.00085	0.055	25	25	80	0.8	0.4
950	0.00082	0.09	50	55	190	0.85	0.43

Temperature		Decomposition rate constants (sec ⁻¹)					
(°C)	(1/K)	k_1'	k_2'	k_3'	k_4'	k_5'	k_6'
800	0.00093	0.001	0.1	0.1	0.05	0.03	0.03
900	0.00085	0.01	3	0.3	0.2	0.07	0.07
950	0.00082	0.03	15	0.5	0.3	0.1	0.1

21