

TABLE VI. Predicted Nitrite and Nitrate Concentrations in Simulation of Experiment EC-237 of the Statewide Air Pollution Research Center of the University of California, Riverside, using the Chemical Mechanism of Falls and Seinfeld (1978)

	Concentration, ppm		
	60 min	180 min	300 min
HONO	0.0061	0.00040	0.00036
HONO ₂	0.067	0.22	0.29
HO ₂ NO ₂	0.00083	0.0019	0.0025
RONO	0.0030	0.00054	0.000080
RONO ₂	0.0041	0.0070	0.0072
$\overset{\text{O}}{\parallel}$ RCOONO ₂	0.025	0.089	0.13
RO ₂ NO ₂	0.034	0.075	0.098

Conditions of the experiment: $T = 303^{\circ}\text{K}$, $k_2 = 0.3 \text{ min}^{-1}$, $[\text{NO}_2]_0 = 0.106$, $[\text{NO}]_0 = 0.377$, $[\text{H}_2\text{O}] = 2.4 \times 10^4$, $[\text{CO}] = 0.96$, $[\text{Aldehydes}]_0 = 0.0012$, $[\text{Alkanes}]_0 = 2.488$, $[\text{Non-ethylene Olefins}]_0 = 0.15$, $[\text{C}_2\text{H}_4]_0 = 0.875$, $[\text{Aromatics}]_0 = 0.177$, $[\text{HONO}]_0$ (assumed) = 0.1 (all concentrations in ppm). Dilution rate = $2.93 \times 10^{-4} \text{ min}^{-1}$.

Like HONO, HO₂NO₂ and RONO, PAN undergoes both formation and decomposition steps (reaction 71). Unlike these former species, however, the balance between the formation and decomposition reactions is such that PAN may achieve appreciable concentration levels relative to those of NO and NO₂. Because the decomposition reaction for PAN is strongly temperature dependent, the steady state PAN concentration is highly dependent on the temperature. As temperature increases the role of PAN as an NO₂ sink decreases markedly; at low temperatures, on the other hand, steady state PAN concentrations can reach rather substantial levels.