

NITRITE AND NITRATE FORMATION

The oxides of nitrogen are converted eventually to nitrites and nitrates by the reactions previously given. In particular, the following gaseous nitrites and nitrates have been identified:

HONO	nitrous acid
HONO ₂	nitric acid
HO ₂ NO ₂	peroxynitric acid
RONO	alkyl nitrite
RONO ₂	alkyl nitrate
$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOONO}_2 \end{array}$	peroxyacetyl nitrate (PAN)
RO ₂ NO ₂	peroxyalkyl nitrate
$\begin{array}{c} \text{O} \\ \parallel \\ \phi\text{C}-\text{OO}-\text{NO}_2 \end{array}$	peroxybenzoyl nitrate (PBZN)

In addition to these gaseous species, particulate nitrites and nitrates may be formed. The object of this section is to present estimates of the importance of the various nitrites and nitrates. In most cases, estimates are necessary because ambient measurements of the concentration level of all but a very few of the species are lacking.

Typical ambient concentration levels of the gaseous nitrogen-containing species listed above can be estimated from simulations of smog chamber experiments using chemical mechanisms representing the hydrocarbon-NO_x chemistry. Table VI lists calculated concentrations of HONO, HONO₂, HO₂NO₂, RONO, RONO₂, RC(O)OONO₂, and RO₂NO₂ for smog chamber experiment EC-237 carried out at the Statewide Air Pollution Research Center of the University of California, Riverside, using the chemical mechanism of Falls and Seinfeld (1978). The conditions of the experiment are given in the footnote of Table VI. The simulated and predicted concentrations of the major measured species, such as NO, NO₂, O₃, PAN, and hydrocarbons, agreed well.