Geophysical Research Abstracts
Vol. 12, EGU2010-11284, 2010
EGU General Assembly 2010

Theoretical studies of the adsorption of hydrogen peroxide and methyl hydroperoxide on ice particles

Stanislav K. Ignatov (1,2), Michael Gand (1), Alexey G. Razuvaev (2), and Otto Schrems (1)

(1) Alfred Wegener Institute for Polar and Marine Research, Climate System, Bremerhaven, Germany (Otto.Schrems@awi.de, +49 471 48311425), (2) N. I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia

The uptake of atmospheric trace gases on microcrystalline water ice particles in the Earth atmosphere is an important process providing the basis of many key reactions which usually do not take place under purely gas-phase conditions.
We have studied the low-temperature interaction between hydrogen peroxide (H2O2) and methyl hydroperoxide (CH3OOH) with hexagonal water ice surfaces by means of DFT (BLYP/6-31++G(d,p)) calculations. The adsorption processes of inorganic and organic peroxides among which hydrogen peroxide and methyl hydroperoxide are the most abundant are very interesting since they are strong oxidants. In our studies we have calculated the structures, energies, and some thermodynamic properties of the molecular surface complexes formed by H2O2 and CH3OOH with water clusters representing the surface fragments of the (0001), (10-10), and (11-20) crystallographic planes of the hexagonal oxygen lattice of the water ice Ih with proton ordering corresponding to Pisani's P-ordered model. The various modes of coordination and intrusion were studied using the extensive set (up to 192 points for each plane) of the structures optimized at the semiempirical (PM3) level. The validity of the surface models was approved by the stability of the results obtained in a (H2O)n cluster series, (n=48, 72, 192, 216) at semiempirical level as well as by DFT calculations of selected structures at the BLYP/6-311++G(2d,2p) level.