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INTERACTION OF HCl WITH A beta-NAT SURFACE: PREDICTION OF THE IR SPECTRUM

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Heterogeneous reactions that take place over the surface of polar stratospheric cloud (PSC) particles are thought to play an important role on stratospheric ozone depletion. Chlorine reservoir species, such as HCl and $ClONO_2$, adsorbed on those particles, can be converted to reactive chlorine compounds, responsible for the destruction of ozone. The high temperature phase of nitric acid trihydrate (β-NAT) is one of the most important constituents of PSC.

We present here a theoretical study of the system formed by HCl and β-NAT, by means of DFT calculations[1]. The adsorption of HCl on the most favourable site of the (001) surface of the β-NAT crystal[2] is simulated with a suitable model for the description of the vibrational properties of the system. Other possible adsorption sites will also be revised. An assignment of the different spectroscopic features, such as a small band at 2150 cm^{-1} attributed to the stretching of the adsorbed HCl molecule, is performed by comparing the predicted absorption spectrum with the experimental results[3]

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