Adsorption of 2,4,6-Trichlorophenol on Kaolinite: *Ab Initio* Calculations of Molecular Models

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2,4,6-Trichlorophenol (TCP) was widely studied experimentally since it's the one of the most wide-spread pollutants, in fact it is used as an insecticide, fungicide, herbicide, bactericide and as a chemical intermediate for the synthesis of other pesticides. So this study is dedicated to investigate the mechanism of adsorption of this compound on the surface of mineral fragment of kaolinite using a two-layered ONIOM approach.

The representative cluster models of the tetrahedral and octahedral surface of kaolinite (1:1type layered silicates) were constructed using its structural data $Al_2Si_2O_5(OH)_4$. The model consists of 78 atoms and contains one tetrahedral ring and one octahedral ring. The resulting chemical formula is $Al_6Si_6O_{36}H_{30}$ .The dangling bonds of the mineral fragment were saturated by the hydrogen atoms, such a model of the mineral is electroneutral.

The calculations were carried out at the *ab initio*; Hartree Fock level and DFT using the standard 6-31G*, 6-31G** basis set of the GAUSSIAN-09 program. The geometry optimization was performed using the two levels ONIOM method (*n*-layered integrated molecular orbital and molecular mechanics approach). The location of the six hydrogen atoms of the outer-OH groups and the geometry of the adsorbed molecule were optimized. In the case of adsorption on the tetrahedral side of the kaolinite layer the geometry of the mineral fragment was kept frozen.

The study reveals that the adsorption TCP on the surface of kaolinite results in polarization and in changes in the geometric parameters of adsorbed molecule and through the formation of multiple hydrogen bonds.