ETHYLENEDIAMINE AT AIR/LIQUID AND AIR/SILICA INTERFACES: PROTONATION VERSUS HYDROGEN BONDING INVESTIGATED BY SUM FREQUENCY SPECTROSCOPY

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The adsorption process on mineral oxide surfaces is one of the most important factors influencing the migration and distribution of the contaminants in the soil environment. Although there are numerous studies carried out at the macroscopic scale, there is lack of molecular scale (microscopic) information at the interfaces. The molecular scale information is often crucial for the determination of sorption mechanisms. In this study, sum frequency generation spectroscopy (SFG), a surface specificvibrational spectroscopy, has been employed to investigate the adsorption of ethylenediamine ($H_2N(CH_2)_2NH_2$, EDA) onto the amorphous SiO_2 surface, and EDA protonated products at air/liquid interfaces. The SFG spectra of EDA adsorbed on the silica surface and the singly protonated EDA solution are similar in both C-H and N-H stretching regions. This indicates EDA molecules are strongly chemisorbed to the silica surface through the protonation of one EDA amino group by surface silanol OH groups, thereby forming a $H_2N(CH_2)_2NH_3$-O-Si surface complex. The SFG results also suggest that the surface acidity of the silanol OH groups (pK_a) is between the two pKa values of EDA (in the range of 7.56 to 10.71) at the air/silica interface.