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**First principles calculations of enthalpy and O-H stretching frequency of hydrogen-bonded acid-base complexes**[1] MESFIN TSIGE, RAM BHATTA, ALI DHINOJWALA, The University of Akron — Understanding the acid-base interactions is important in surface science as it helps to rationalize materials properties such as wetting, adhesion and tribology. Quantitative relation between changes in enthalpy (ΔH) and frequency shift ($\Delta\nu$) during the acid base interaction is particularly important. We investigate ΔH and $\Delta\nu$ of twenty-five complexes of acids (methanol, ethanol, propanol, butanol and phenol) with bases (benzene, pyridine, DMSO, $Et_2O$ and THF) in $CCl_4$ using intermolecular perturbation theory calculations. ΔH and $\Delta\nu$ of complexes of all alcohols with bases except benzene fall in the range from -14 kJ/mol to -28 kJ/mol and 215 $cm^{-1}$ to 523 cm$^-$1, respectively. Smaller values of ΔH (-2 to -6 kJ/mol) and $\Delta\nu$ (23 to 70 $cm^{-1}$) are estimated for benzene. For all the studied complexes, ΔH varies linearly ($R^2$ ? 0.974) with $\Delta\nu$ yielding the average slope and intercept of 0.056 and 1.5, respectively. Linear correlations were found between theoretical and experimental values of ΔH as well as $\Delta\nu$ and are concurrent with the Badger-Bauer rule.

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