Investigating the effect of solvent polarity on the IR and NMR spectra of acetone

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IR and NMR are one of the most accurate and powerful experimental techniques at our disposal to study molecules. This sensitivity of these two spectroscopic observables with the surrounding medium (solvent) helps us understand the local electrostatics near the vicinity of the solute due to the external environment. Hence, they play a significant role in modern chemistry as well as in biology. Here, we investigate the sensitivity of these two spectroscopic observables for carbonyl moiety of acetone to the polar solvents. Our quantum chemical calculations have shown that bond polarization of the carbonyl bond happens in the presence of a polar solvent. This picture of bond polarization is used to explain the sensitivity of these spectra. Additionally, to explain the redshift in the IR spectrum of acetone in the presence of an external electric field there are two popular models in literature. One is the vibrational Stark effect (VSE), and another is the bond polarization model. Our study shows that there can be contributions from both models to the IR redshifts of C=O stretch of acetone and further, the study shows that the contribution due to VSE is around one and a half times more than the bond polarization model.