SOLVENT EFFECTS ON IR MODES OF (R)-3-METHYLCYCLOPENTANONE CONFORMERS: A COMPUTATIONAL INVESTIGATION

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Density Functional Theory (DFT) calculations of infrared spectra for the optimized geometries of R-(+)-3-methylcyclopentanone (R3MCP) equatorial-methyl and axial-methyl conformers were performed in 11 common solvents of wide polarity range, in the framework of polarizable continuum model (PCM). DFT correlation function type B3LYP using a powerful basis set (aug-cc-pVDZ) yielded different linear correlation between solvent polarity and R3MCP equatorial and axial conformers IR modes frequencies, intensities, and enthalpies (W. Al-Basheer, J. Sol. Chem. 41, 1495-1506 (2012)). DFT calculations of the R3MCP equatorial and axial conformer dipole moment components in 3D were also carried out and found to have a linear correlation with solvent polarity (W. Al-Basheer et al, J. Phys. Chem. A 111(12), 2293-2298 (2007)). An observed trend for a Hypsochromic (blue) shift in the equatorial conformer IR frequencies, in comparison to Bathochromic (red) shift for the axial-methyl conformer IR modes as a function of solvent polarity increase.