Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Sensitivity of chiral 3-methylcyclopentanone structure, electric moment and thermodynamic parameters to medium polarity WATHEQ AL-BASHEER, Department of Physics, King Fahd University of Petroleum & Minerals, SAID AL AZAR, Basic Sciences Department, Dar Al Uloom University — *R*-(+)-3-methylcyclopentanone (*R*3MCP) is a chiral ketone which can exist in as many as five conformers with two dominant conformers at room temperature; equatorial-methyl and axial-methyl. Density Functional Theory (DFT) calculations of the optimized geometries of *R*-(+)-3-methylcyclopentanone (*R*3MCP) individual dominant conformers were performed in 10 common solvents of wide polarity range, under 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 *R*3MCP equatorial and axial conformers Gibbs free and zero-point energies, entropies, vibrational modes frequencies, in addition to heat capacity resulting from translational, electronic, rotational and vibrational motion. Furthermore, DFT calculations of the *R*3MCP equatorial and axial conformers electric dipole and quadrupole moments components in 3D were also carried out and found to have a linear correlation with solvent polarity and cavitation energy. An observed trend for the standard Gibbs energies for the rotational equilibrium of *R*3MCP to be strongly-solvent dependent will be presented.

Watheq Al-Basheer
King Fahd University of Petroleum & Minerals

Date submitted: 12 Nov 2014 Electronic form version 1.4