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Chemical structure-optical property understanding in bisphenyls and substituted polycarbonates by molecular simulations: Role of polarizabilities and conformations UPENDRA NATARAJAN, National Chem. Lab. India, M.S. SULATHA, National Chem. Lab. India — We present calculations of polarizability tensors, optical anisotropy of organic molecules, repeating units and polymer chains of several bisphenyls, bisphenol carbonates and polycarbonates with a variety of chemical substitutions.[1,2] Theoretical calculations of polarizabilities and optical birefringence of several newer structures having specific side-group substitutions which render low birefringence, not previously reported, is also shown here. Our method combines VOSRIS scheme[3], molecular geometry and conformations from force-field simulations and accurate anisotropic polarizability tensors. Aliphatic, aliphatic aromatic and cycloaliphatic substitutions reduce optical anisotropy in relation to bisphenol A polycarbonate. Calculated $\langle\gamma^2\rangle/x$ of these structurally modified polycarbonates[2] follows linear behavior with respect to experimentally observed melt stress-optical coefficient (C_m).

1. *J. Phys. Chem. A*, **107**, 97 (2003)

2. *Macromolecules*, **36**, 2944 (2003)

3. P.J. Flory, *Statistical Mechanics of Chain Molecules*, Wiley Interscience, New York (1969)

Upendra Natarajan
National Chem. Lab. India

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