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Influence of number and position of nitro groups in tuning the thermodynamic and nonlinear optical properties of ethylenediaminium nitrophenolates

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Abstract

Estimation of thermodynamic and third-order nonlinear optical properties of a series of organic liquids based on ethylenediaminium divalent cation, $[C_2H_{10}N_2]X_2$ (where X = 2-nitrophenol, 4-nitrophenol, 2,4-dinitrophenol and 2,4,6-trinitrophenol respectively) was made. Increase in nitro groups of ethylenediaminium nitrophenolates has predominantly increased the point of decomposition (145-243 °C). Various thermodynamic properties as a function of temperature were estimated theoretically from the DSC curves. Thermal conductivity and specific heat capacity was increasing while thermal diffusivity was decreasing with rise in temperature. Ethylenediaminium trinitrophenolate (EDA246TNP) showed maximum thermal conductivity ($30.3 \text{ W m}^{-1} \text{ K}^{-1}$) and specific heat capacity ($2684 \text{ J K}^{-1} \text{ K}^{-1}$), while thermal diffusivity ($9.6 \times 10^{-6} \text{ m}^2 \text{ S}^{-1}$) was higher for ethylenediaminium 2-nitrophenolate (EDA2NP). Z-scan experiment showed that all samples exhibit saturable absorption and self-defocusing behaviour under CW laser (532 nm, 50 mW) excitation. The observed nonlinearity was found to be thermal in origin with order of nonlinearity as ED246TNP>EDA24DNP> EDA4NP>EDA2NP. EDA246TNP possess maximum nonlinear absorption coefficient ($8.37 \times 10^{-3} \text{ cm/W}$), nonlinear refractive index ($8.41 \times 10^{-8} \text{ cm}^2/\text{W}$), third-order nonlinear optical susceptibility ($5.21 \times 10^{-6} \text{ esu}$), second-order hyperpolarizability ($9.81 \times 10^{-25} \text{ esu}$) and thermo-optic coefficient ($-0.21 \times 10^{-6} \text{ K}^{-1}$) than other phenol-ammonium salts. All samples exhibit optical limiting action with optical limiting onset values of 35-38 mW having limiting amplitude of 6.7-9.3 mW. The influence of number and position of nitro groups in tuning the thermodynamic and nonlinearity of ethylenediaminium nitrophenolate was discussed in detail.

Keywords: Organic, NLO, Thermodynamic, Z-scan, Optical limiting

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