**Design of Organic Chromphore with Head-to-Tail Molecular Dipole Alignment for SHG (Calibri(Body) 14 font bold)**

**Ravindra H J1\*** & S M Dharmaprakash2 **(12 font, Presenting author (Bold)**

1Dept. of Physics, Shri Madhwa Vadiraja Institute of Technology and Management, Bantkal, Udupi-574115

2Dept. of Physics, Mangalore University, Mangalagangothri, Konaje -574119

\*E-mail: ravi23911@gmail.com **(Affiliation 10 font)**

**Abstract (12 font bold)**

Single crystals of a chalcone co-crystal (C18H19NO4/C17H16NO3Br; 0.972/0.028) have been grown by slow evaporation from solution. The powder second harmonic generation (SHG) efficiency of this chalcone co-crystal is 7 times that of urea. The dependence of second harmonic (SH) intensity on particle size revealed the existence of phase matching direction in this crystal. The large SHG efficiency observed is mainly due to the unidirectional alignment of molecular dipoles, in which the dipole moment of each molecule adds to establish a net polarization. The weak N–H⋅⋅⋅O hydrogen-bond interactions help to stabilize the noncentrosymmetric crystal packing and also contribute partly to the SHG. The better thermal stability, transparency and high laser damage resistance (>1.5 GW cm−2 at 532 nm, 8 ns) of this chalcone co-crystal indicate that it is a promising material for frequency doubling of diode lasers down to 470 nm. This molecule also shows a third-order NLO response and good optical limiting property of 8 ns laser pulses at 532 nm. The mechanism for optical limiting in this chalcone was attributed to two-photon induced excited state absorption that leads to reverse saturable absorption. The structure–property relationship in this chalcone and related compounds is discussed based on the experimental results and semiempherical hyperpolarizability calculations.

**Keywords**: Organic material, Second harmonic generation, co-crystal, crystal structure

**(Running text: 11 font, 1.15 line spacing, abstract of the research article maximum of one page)**