JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 51 (2018)

Supporting information for article:

Crystal growth and characterization of second-and third-order nonlinear optical chalcone derivative: (2E)-3-(5-Bromo-2-thienyl)-1-(4-nitrophenyl)-prop-2-en-1-one

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Z-scan method:

Single beam Z-scan readily gives the magnitude and sign of the nonlinearity (Sheik-Bahae *et al.*, 1990). The experimental setup used to measure the NLA and NLR index of **5B2SNC** is identical to that described in our previous studies (Patil *et al.,* 2016).The experiment was conducted with sample concentration of 1 mM using femtosecond (fs) pulses emitted from Ti: sapphire laser with a wavelength 800 nm, a pulse duration of 120 fs, and a repetition rate of 80 MHz. It consists of two parts: an open aperture (OA) part, where the total sample transmitted intensity was measured without the aperture as a function of sample position, and a closed aperture (CA) part, where an aperture was placed in front of the detector and only the fraction of intensity passing through the aperture was recorded as a function of the sample position on the Z-axis. CA scans were performed at intensities where the contribution from the higher order nonlinear effects is negligible (the value of $\Delta\phi$ estimated in all the cases was $<\pi$). The experiments were repeated more than once and the best data were used for obtaining the NLO coefficients from the best fits.

Fig. 1S. Powder X-ray diffraction pattern of **5B2SNC**.

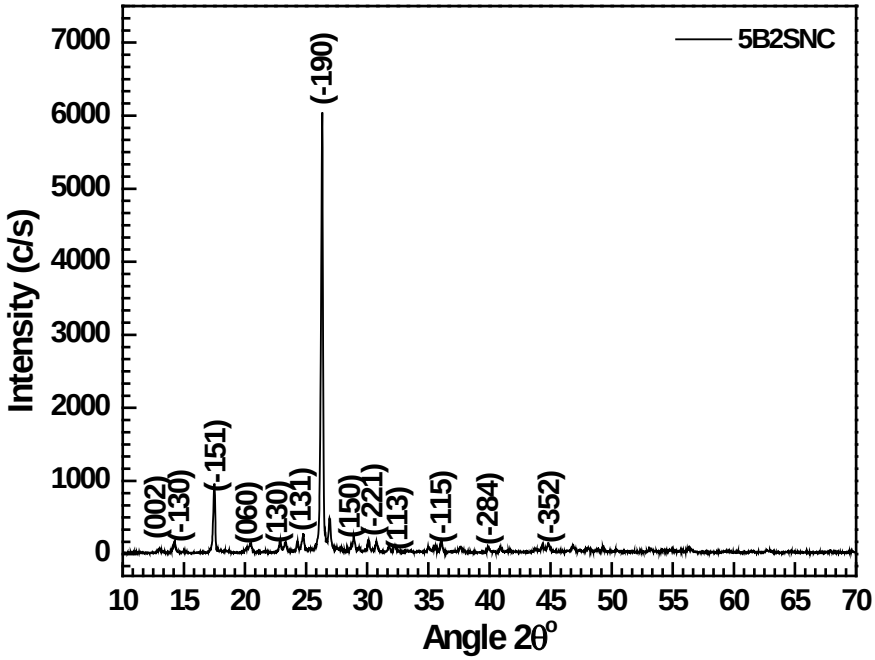

Fig. 2S. TGA/DTA curve of **5B2SNC**.

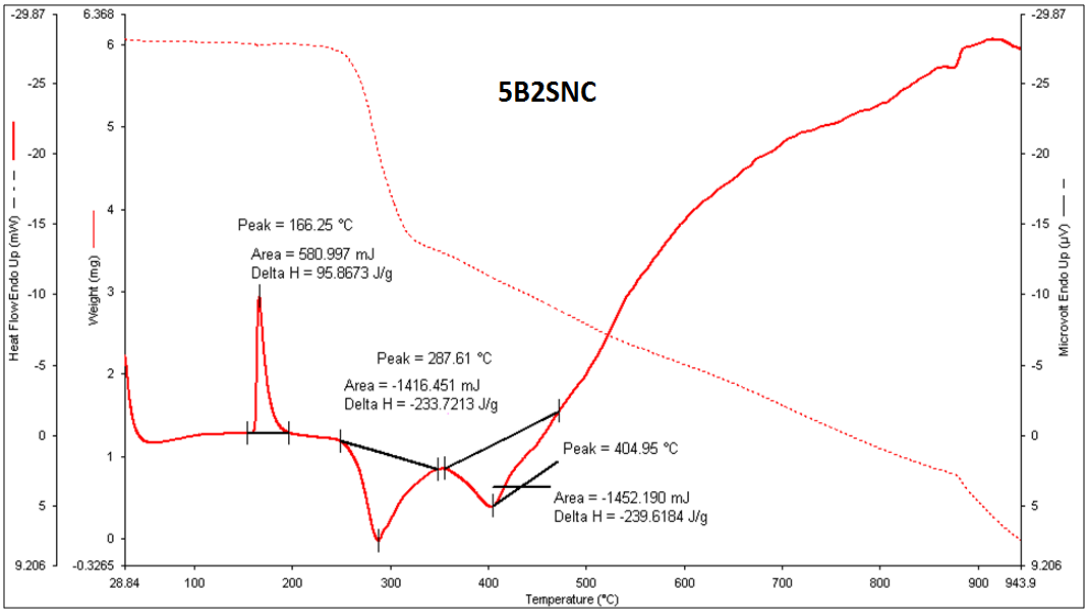

Table 1S

Frontier molecular orbital (FMO) energies and their differences at B3LYP/6-31G* level of theory.

Orbitals	Energy	
	a.u.	eV
E_{HOMO}	-0.235	-6.394
E_{HOMO-1}	-0.265	-7.211
E_{LUMO}	-0.110	-2.993
E_{LUMO+1}	-0.084	-2.285
$\Delta E_{HOMO-LUMO}$	0.125	3.401
$\Delta E_{HOMO-1-LUMO+1}$	0.180	4.898

Table 2S

The values of α, β *and* μ along with their individual tensor components computed at B3LYP/6-31G* level of theory. (For α, 1 a. u. = 0.1482×10^{-24} esu and for β, 1 a. u. = 0.008629×10^{-30} esu).

Polarizability and dipole moment			Hyperpolarizability		
Components	a. u.	esu ($\times10^{-24}$)	Components	a. u.	esu ($\times10^{-30}$)
α_{xx}	*393.96*	*58.38*	β_{xxx}	*-5902.44*	*-50.93*
α_{xy}	*-2.78*	*-0.41*	β_{xxy}	*935.97*	*8.08*
α_{yy}	*199.81*	*29.61*	β_{xyy}	*-167.66*	*-1.45*
α_{xz}	*7.13*	*1.06*	β_{yyy}	*79.40*	*0.69*
α_{yz}	*-5.17*	*-0.77*	β_{xxz}	*40.55*	*0.35*
α_{zz}	*71.77*	*10.64*	β_{xyz}	*-7.44*	*-0.06*
α_0	*221.85*	*32.88*	β_{yyz}	*3.71*	*0.03*
$\Delta\alpha$	*281.30*	*41.69*	β_{xzz}	*10.41*	*0.09*
μ_x	*-5.756D*		β_{yzz}	*-16.40*	*-0.14*
μ_y	*1.456D*		β_{zzz}	*-3.63*	*-0.03*
μ_z	*0.291D*		β_0	*3684.99*	*31.8*
μ_{tot}	*5.944D*		β_{tot}	*6141.66*	*53*

Table 1R The values of α, β *and* μ along with their individual tensor components computed at HF/6-31G* level of theory.

Polarizability and dipole moment			*Hyperpolarizability*		
Components	*a. u.*	*esu* ($\times 10^{-24}$)	*Components*	*a. u.*	*esu* ($\times 10^{-30}$)
α_{xx}	*358.14*	*53.08*	β_{xxx}	*-4646.97*	*-40.1*
α_{xy}	*-1.06*	*-0.16*	β_{xxy}	*865.57*	*7.47*
α_{yy}	*190.85*	*28.28*	β_{xyy}	*-161.70*	*-1.39*
α_{xz}	*12.06*	*1.79*	β_{yyy}	*94.62*	*0.82*
α_{yz}	*-6.54*	*-0.97*	β_{xxz}	*45.65*	*0.39*
α_{zz}	*76.67*	*11.36*	β_{xyz}	*-3.13*	*-0.03*
α_{0}	*208.55*	*30.91*	β_{yyz}	*4.37*	*0.04*
$\Delta\alpha$	*245.19*	*36.34*	β_{xzz}	*8.84*	*0.08*
μ_x	*-5.072D*		β_{yzz}	*-11.30*	*-0.10*
μ_y	*1.087D*		β_{zzz}	*-6. 37*	*-0.05*
μ_z	*0.215D*		β_{0}	*2367.45*	*20.43*
μ_{tot}	*5.192D*		β_{tot}	*3945.75*	*34.05*

Table 2R The values of α, β *and* μ along with their individual tensor components computed at CAM-B3LYP/6-31G* level of theory.

Polarizability and dipole moment			*Hyperpolarizability*		
Components	*a. u.*	*esu* ($\times 10^{-24}$)	*Components*	*a. u.*	*esu* ($\times 10^{-30}$)
α_{xx}	*348.69*	*51.68*	β_{xxx}	*-3639.62*	*-31.41*
α_{xy}	*-1.45*	*-0.21*	β_{xxy}	*736.25*	*6.35*
α_{yy}	*193.74*	*28.71*	β_{xyy}	*-113.48*	*-0.98*
α_{xz}	*7.34*	*1.09*	β_{yyy}	*83.23*	*0.72*
α_{yz}	*-4.91*	*-0.73*	β_{xxz}	*25.41*	*0.22*
α_{zz}	*71.28*	*10.56*	β_{xyz}	*-5.60*	*-0.05*
α_{0}	*204.57*	*30.32*	β_{yyz}	*2.13*	*0.02*
$\Delta\alpha$	*241.13*	*35.74*	β_{xzz}	*9.87*	*0.09*
μ_x	*-5.174D*		β_{yzz}	*-15.73*	*-0.14*
μ_y	*1.078D*		β_{zzz}	*-4.17*	*-0.04*
μ_z	*0.138D*		β_{0}	*1811.34*	*15.63*
μ_{tot}	*5.287D*		β_{tot}	*3018.90*	*26.05*

Table 3R The values of α, β *and* μ along with their individual tensor components computed at wb97XD/6-31G* level of theory.

Polarizability and dipole moment			*Hyperpolarizability*		
Components	*a. u.*	*esu* ($\times 10^{-24}$)	*Components*	*a. u.*	*esu* ($\times 10^{-30}$)
α_{xx}	*346.76*	*51.39*	β_{xxx}	*-3366.90*	*-29.05*
α_{xy}	*-1.16*	*-0.17*	β_{xxy}	*703.41*	*6.07*
α_{yy}	*193.16*	*28.63*	β_{xyy}	*-120.63*	*-1.04*
α_{xz}	*11.36*	*1.68*	β_{yyy}	*82.53*	*0.71*
α_{yz}	*-5.89*	*-0.87*	β_{xxz}	*22.65*	*0.2*
α_{zz}	*75.52*	*11.19*	β_{xyz}	*-1.20*	*-0.01*
α_0	*205.15*	*30.4*	β_{yyz}	*4.99*	*0.04*
$\Delta\alpha$	*236.41*	*35.04*	β_{xzz}	*12.70*	*0.11*
μ_x	*-5.184D*		β_{yzz}	*-13.07*	*-0.11*
μ_y	*1.135D*		β_{zzz}	*-4.53*	*-0.04*
μ_z	*0.220D*		β_0	*1671.35*	*14.42*
μ_{tot}	*5.311D*		β_{tot}	*2785.58*	*24.04*

Figure 3S Comparison of first hyperpolarizability calculated at different levels of theory with urea molecule (urea value at B3LYP/6-31G*)