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Supporting information for article:

2,2′-(Disulfanediylbis{5-[(1*E*)-(2-hydroxybenzylidene)amino]-1,3-thiazole-4,2-diyl})diphenol: synthesis, crystal structure and theoretical evaluation of nonlinear optical property

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A novel Schiff base compound: synthesis, crystal structure and theoretical evaluation of nonlinear optical property

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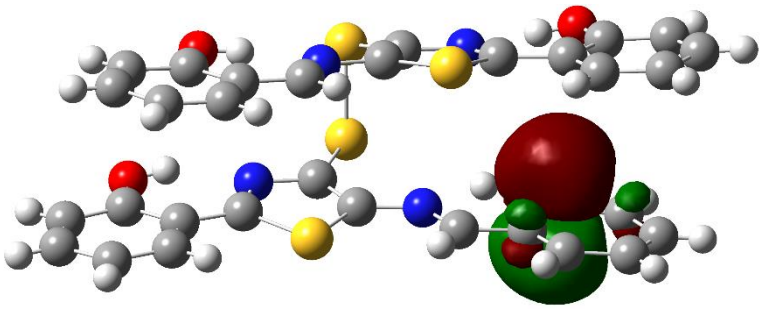
The calculated HOMO and LUMO energies of the compound

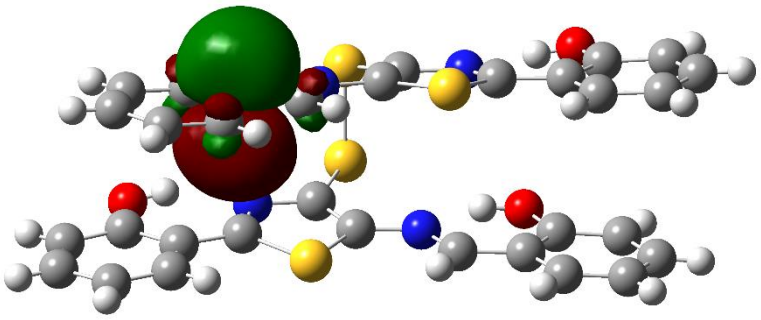
The chemical stability of a molecule can be reflected from the energies of frontier molecular orbitals, i.e. the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies, that have been calculated by means of B3LYP/6-311G(d,p) method and displayed in Fig. 1S.

According to the bond lengths (Table 3), the presence of a π–conjugated system across the skeleton of the synthesized Schiff base compound can be concluded. This π–conjugated system can undertake the ease electronic communication between the HOMO and LUMO (Fig 1S) in the synthesized Schiff base compound and act as the basis of intramolecular charge transfer. The low value of the calculated LUMO-HOMO energy gap and the high value of the calculated dipole moment of the synthesized Schiff base compound can signify the intramolecular charge transfer that is responsible the magnitude of the molecular properties.



E_{LUMO} = - 3.1446 eV

ΔE = 0.0284 eV



E_{HOMO} = - 3.1730 eV

Figure 1S

The calculated frontier molecular orbitals plots at B3LYP/6-311G(d,p) level.

Second-order nonlinear optical calculation

$\alpha = 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$,

$\Delta\alpha = 2^{-1/2}[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{xx} - \alpha_{zz})^2 + (\alpha_{yy} - \alpha_{zz})^2]^{1/2}$,

and $\beta = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$

where

$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$

$\beta y = \beta_{yyy} + \beta_{yzz} + \beta_{xxy}$

$\beta z = \beta_{xxz} + \beta_{yyz} + \beta_{zzz}$

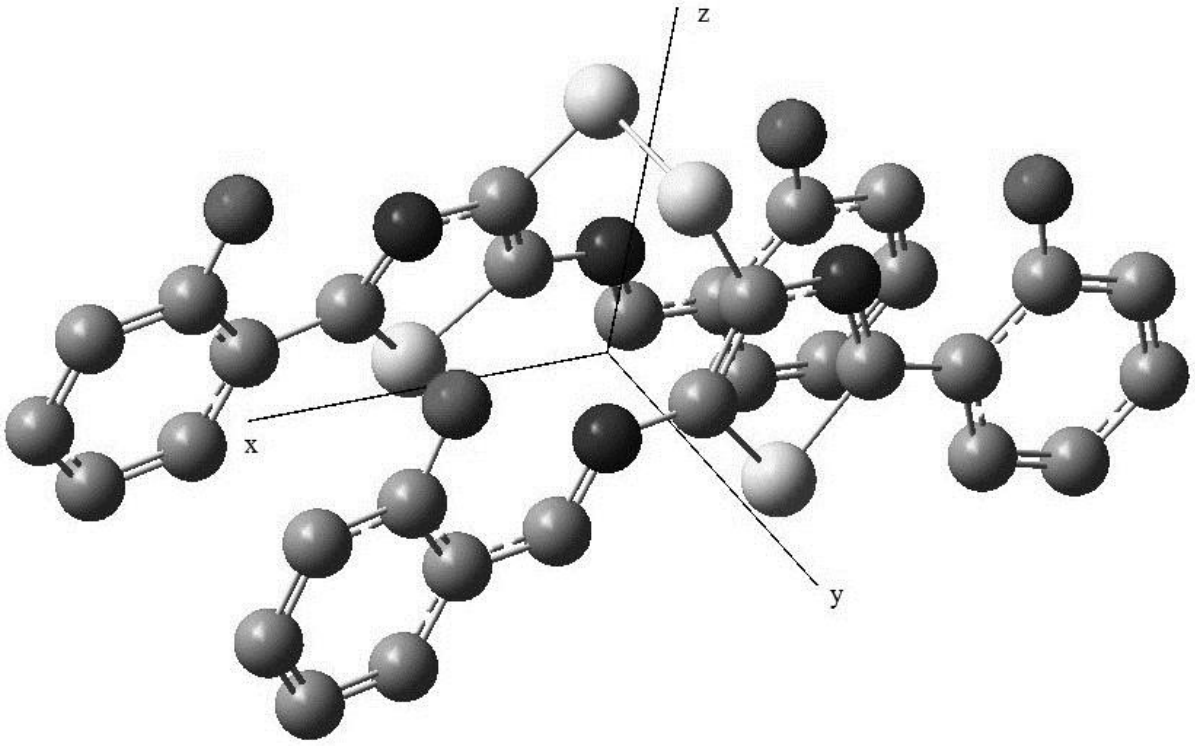


Figure 2S

The orientation of Cartesian directions in calculation of nonlinear optical parameters (The hydrogen atoms omitted).

Table 1S

Calculated values of polarizability ($\times 10^{-24}$ esu) and hyperpolarizability ($\times 10^{-30}$ esu) parameters using DFT/B3LYP/6-311G(d,p) method for the synthesized Schiff base compound.

Polarizability parameters	Value (esu)	Hyperpolarizability Parameters	Value (esu)
α_{xx}	82.26	β_{xxx}	-0.05
α_{xy}	0	β_{xxy}	-4.84
α_{yy}	59.29	β_{xyy}	-0.19
α_{xz}	43.21	β_{yyy}	-2.14
α_{yz}	0	β_{xxz}	-0.02

α_{zz}	72.63	β_{xyz}	-3.28
α	71.39	β_{yyz}	0.01
$\Delta\alpha$	20.03	β_{xzz}	-0.01
		β_{yzz}	-1.82
		β_{zzz}	0.04
		β	8.80

Figure 1S The calculated frontier molecular orbitals plots at B3LYP/6-311G(d,p) level

Figure 2S The orientation of Cartesian directions in calculation of nonlinear optical parameters (The hydrogen atoms omitted)