**Synthesis and DFT calculations of linear and nonlinear optical responses of novel 2-thioxo-3-N,(4-methylphenyl) thiazolidine-4 one**

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**Table S1.** The coordinates of the minimized structure of the 2–thioxo–3–N, (4–methylphenyl) thiazolidine–4–one obtained at B3LYP/6–311+G(d,p) level.

*---------------------------------------------------------------------*

 *Atom Type Coordinates (Angstroms)*

 *X Y Z*

 *---------------------------------------------------------------------*

 *C 1.40359100 -1.57164300 0.00073500*

 *C 1.63500700 0.81070800 -0.00037800*

 *N 0.80290500 -0.30269300 0.00035700*

 *C -0.63567500 -0.18554300 0.00047400*

 *C -1.32313600 -0.13825600 1.20737400*

 *C -1.32361200 -0.14227700 -1.20670800*

 *C -2.71114400 -0.04154100 1.20101100*

 *H -0.77655000 -0.16895500 2.14234700*

 *C -2.71124700 -0.04561700 -1.20036600*

 *H -0.77713100 -0.17615400 -2.14163800*

 *C -3.42775900 0.00444400 0.00049100*

 *H -3.24390700 0.00141400 2.14499000*

 *H -3.24427000 -0.00600500 -2.14440800*

 *C -4.93486400 0.07965300 -0.00062800*

 *H -5.37453600 -0.92282400 -0.04142800*

 *H -5.31033500 0.56598500 0.90223400*

 *H -5.30532900 0.63472400 -0.86539900*

 *O 0.79579000 -2.61148500 0.00119200*

 *S 1.17178200 2.38305000 -0.00118000*

 *C 2.91966900 -1.46458000 0.00050000*

 *H 3.31332300 -1.96193000 -0.88667600*

 *H 3.31351600 -1.96110400 0.88805400*

 *S 3.33281700 0.31529300 -0.00039100*

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**Figure S1.** The optimized molecular geometry of the 2–thioxo–3–N, (4–methylphenyl) thiazolidine–4–one obtained at B3LYP/6–311+G(d,p) level.

**The calculation details:**

We provided a full sheet for calculated values of , their full expressions can be find in Ref. [43]:

We calculate the orientational averages of the tensor components and

For the invariant :

For the invariant :

after, we detail each sum separately:

The invariant :

 *=*

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and the same for the second term .

**Table S2.** First hyperpolarizability β contributions and the gas phase EFISHG obtained using eight DFT functionals at 6–311+G(d,p) basis set.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | B3LYP | PBE0 | B3PW91 | CAM–B3LYP | ωB97X–D | M06 | M05–2X | M06–2X |
|  | 97.87 | 221.66 | 106.52 | 9.59 | 19.66 | 100.19 | 15.058 | 8.15 |
|  | 194.49 | 191.66 | 190.44 | 197.93 | 207.64 | 188.67 | 198.64 | 199.53 |
|  | 248.73 | 277.85 | 239.44 | 228.69 | 227.35 | 249.48 | 214.07 | 220.36 |
|  | 14.29 | -1.58 | 13.80 | 27.19 | 46.28 | 34.20 | 50.75 | 33.05 |
|  | -0.22 | -0.13 | -0.10 | -0.13 | -0.08 | -0.12 | -0.24 | -0.09 |
|  | -0.24 | -0.27 | -0.24 | -0.23 | -0.22 | -0.31 | -0.16 | -0.23 |
|  | -0.94 | -0.97 | -0.96 | -0.89 | -0.95 | -0.72 | -1.10 | -0.85 |
|  | -2.46 | -5.55 | -5.66 | -3.82 | -1.56 | -18.27 | -1.150 | -16.25 |
|  | 58.00 | 59.46 | 54.89 | 52.93 | 57.63 | 58.02 | 55.93 | 45.40 |
|  | 1.08 | 1.08 | 1.07 | 1.04 | 1.08 | 0.74 | 0.85 | 0.78 |
|  | –234.24 | –281.34 | –230.17 | –208.71 | –228.24 | –234.27 | –223.59 | –204.66 |

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**Figure S2.** Optical absorbance spectra for the 2–thioxo–3–N, (4–methylphenyl) thiazolidine–4–one.



**Figure S3.** 1H NMR spectrum for the 2–thioxo–3–N, (4–methylphenyl) thiazolidine–4–one.


**Figure S4.** Spread of 7 to 7.75 ppm (AB system).

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**Figure S5.** 13C NMR spectrum for the 2–thioxo–3–N, (4–methylphenyl) thiazolidine–4–one.