Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary material for the article "**STRUCTURAL, VIBRATIONAL AND ELECTRONIC CHARACTERIZATION OF 1-BENZYL-3-FUROYL-1-PHENYLTHIOUREA: AN EXPERIMENTAL AND THEORETICAL STUDY"** by María Eliana DefonsiLestard[1,*,+], Diego M. Gil[1], Osvaldo Estévez-Hernández[2,3], Mauricio F. Erben[4] and J. Duque[2,3]

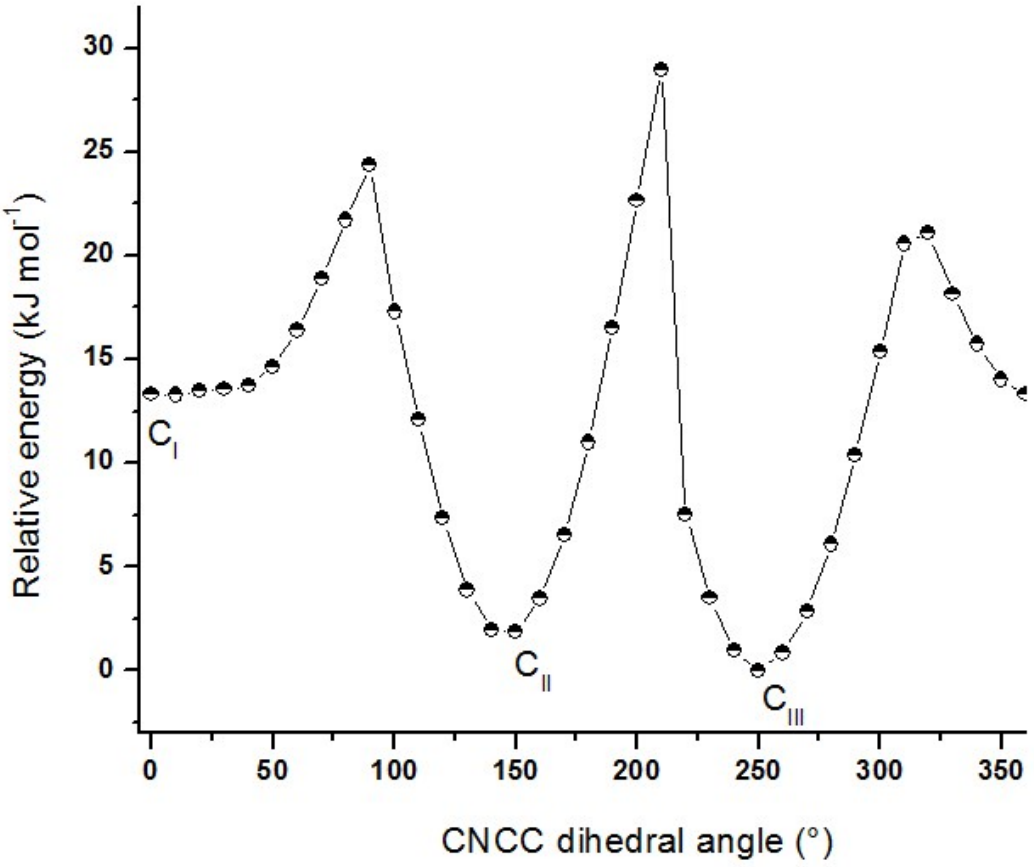

Figure S1: B3LYP/6-31G(d,p)-calculated potential energy profile for the internal rotation of N(20)-C(2) bond.

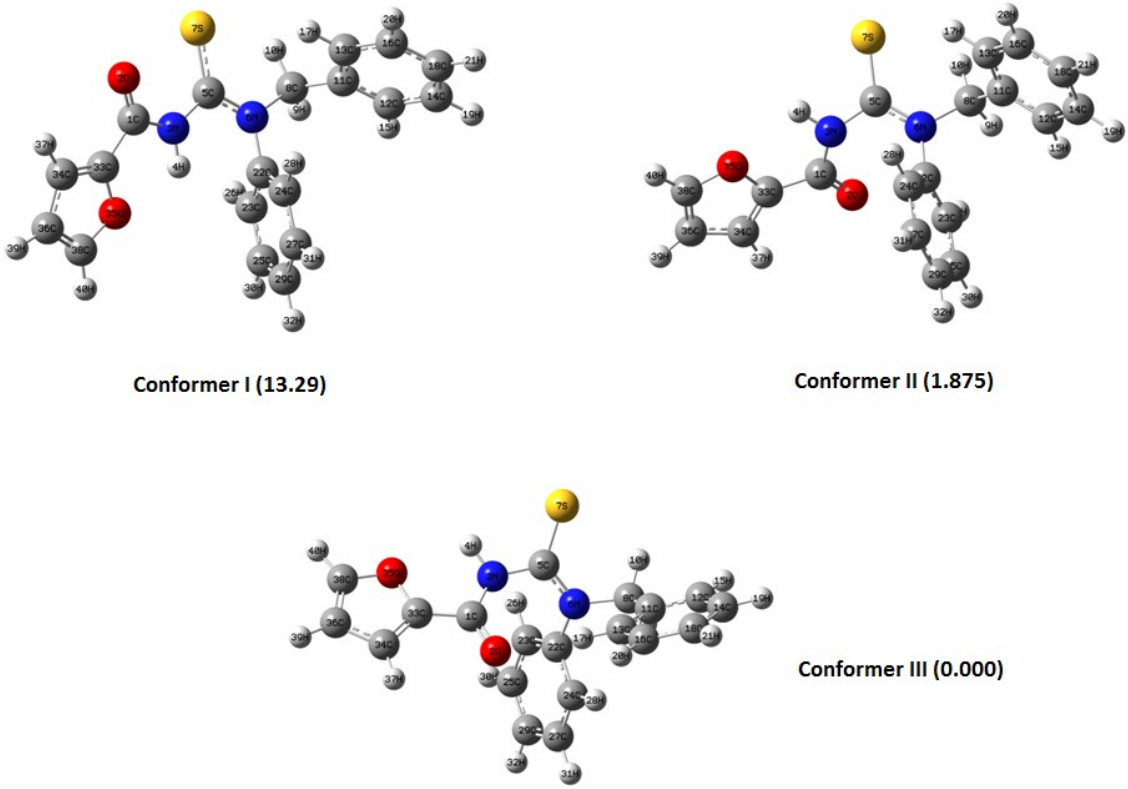

Figure S2: The three low energy stable conformers of 1-benzyl-3-furoyl-1-phenylthiourea. Relative energy values (in kJ mol^{-1}) are given in parenthesis.

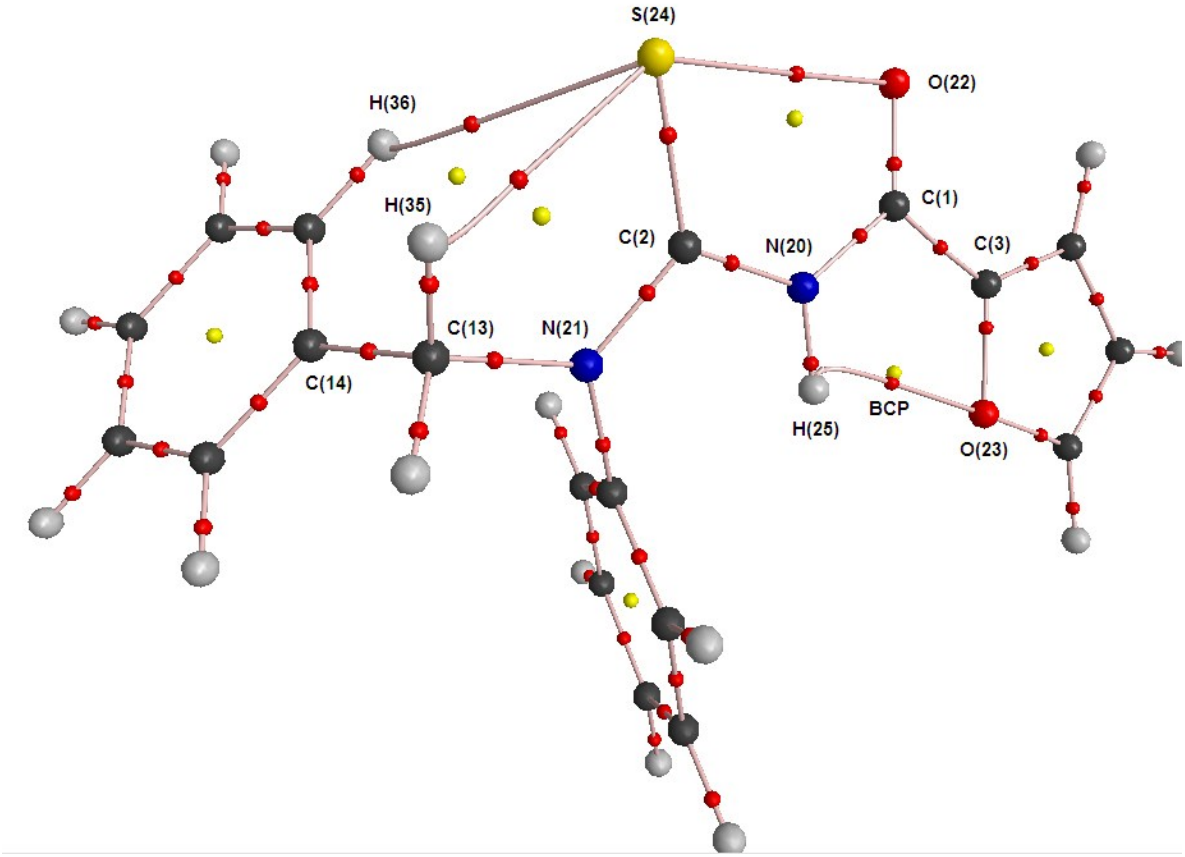

Figure S3: Molecular graph of 1-benzyl-3-furoyl-1-phenylthiourea calculated at B3LYP/6-311++G(d,p) level using AIM program: Bond critical points (small red spheres), ring critical points (small yellow spheres) and bond path (pink lines).

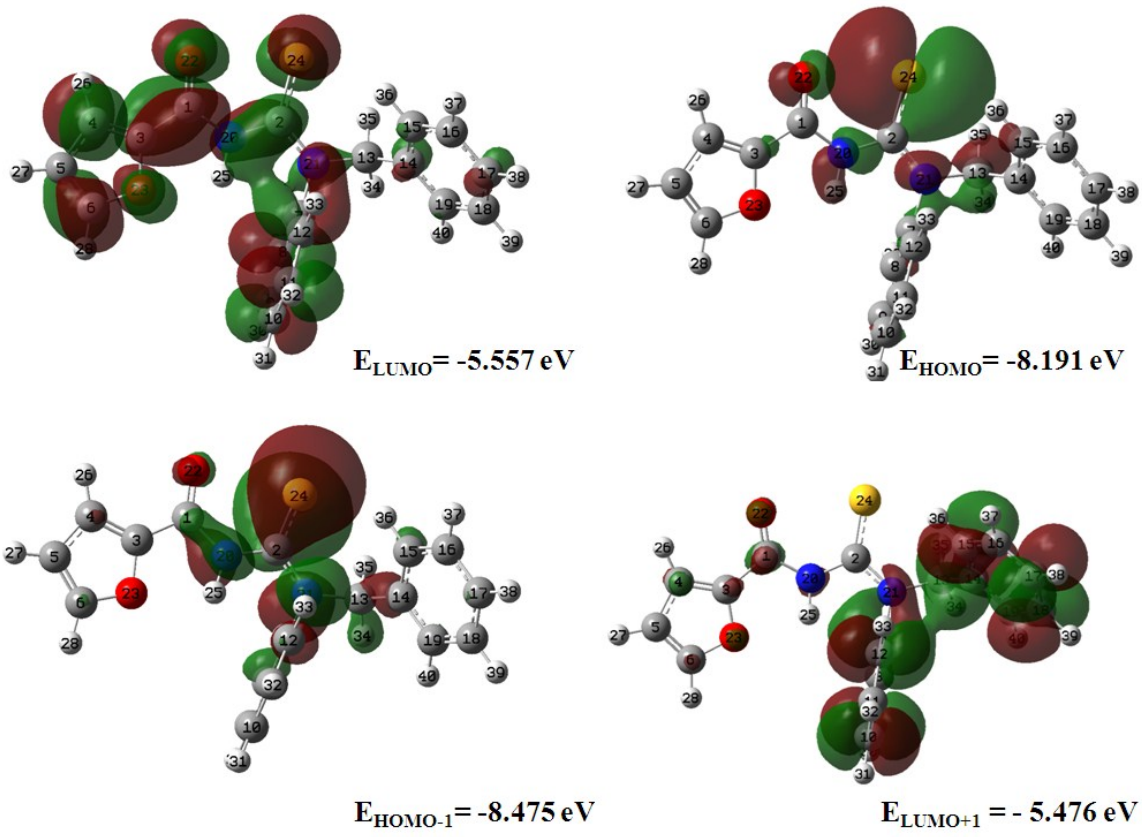

Figure S4: Frontier molecular orbitals HOMO, LUMO, HOMO-1, LUMO+1 for 1-benzyl-3-furoyl-1-phenylthiourea.

Table S1: Dipole moment, polarizability and first-order hyperpolarizability data for 1-benzyl-3-furoyl-1-phenylthiourea calculated at B3LYP/6-311++G(d,p) level of approximation.

Polarizability		First-order hyperpolarizability	
B3LYP/6-311++G(d,p)		B3LYP/6-311++G(d,p)	
α_{xx}	282.254	β_{xxx}	208.651
α_{xy}	16.274	β_{xxy}	-342.485
α_{yy}	216.844	β_{xyy}	-417.551
α_{xz}	-8.922	β_{yyy}	312.550
α_{xz}	21.906	β_{xxz}	-160.014
α_{zz}	302.503	β_{xyz}	-112.348
$\alpha_{mean(a.u.)}$	267.200	β_{yyz}	-358.586
$\alpha_{mean(e.s.u)}$	3.959×10^{-23}	β_{xzz}	-352.773
μ_x	3.0109	β_{yzz}	89.325
μ_y	0.1451	β_{zzz}	603.382
μ_z	-0.609	$\beta_{total\ (a.u)}$	551.546
μ_{total}	3.075	$\beta_{total\ (e.s.u.)}$	4.765×10^{-30}