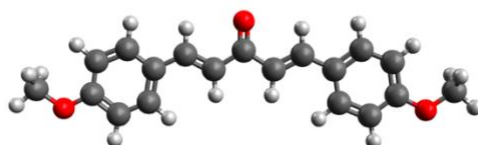
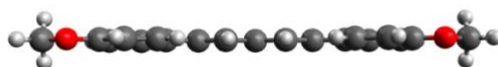
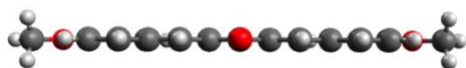
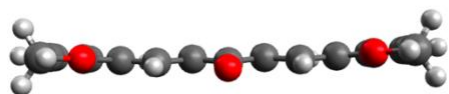


Supplementary Data

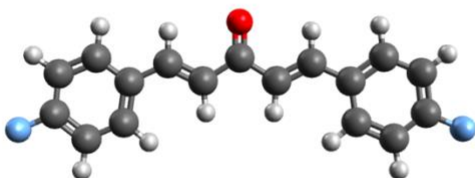
- 3D View from the model molecules' equilibrium geometries: optimized at the CAM-B3LYP/6-311++(2d,p) level of theory using Gaussian.



Molecule: 4-DMDBA



Molecule: 2-DMDBA



Molecule: 4-DFDBA

- Print screen from the post-processing software that is used to calculate the first molecular hyperpolarizability, after the geometry optimization process.

First-Order Hyper Calculator

Post Processing of QCC: Static and Dynamic First-Order Hyperpolarizabilities

Compound Information

New Compound

Modify Compound Information

Open Gaussian Log File

Log File Information

File name: **4dmdba_DCM_Beta_CAMB3LYP.log**
 Calculation status: **OK**
 Terminated in: **Wed Sep 5 23:24:11 2018.**
 Gaussian version: **Gaussian 09, Revision D.01**
 Functional used: **CAM-B3LYP**
 Basis set used: **6-311+G(d,p)**
 Solvent used: **Dichloromethane**
 Theo. wavelength (nm): **1064**

[Show Results](#)

Results

Compound designation: **4-DMDBA**
 Description: **n/info**
 Functional/Basis Set: **CAM-B3LYP / 6-311+G(d,p)**

Molar mass: n/info Theo. molecular mass: n/a
 Chemical formula: n/info Theo. chemical formula: n/a
 Exp. solvent: DCM Theo. solvent: Dichloromethane
 Exp. wavelength (nm): n/info Theo. wavelength (nm): 1064

Formalism	Theoretical		Experimental	Difference (theo-exp)
	Static	Dynamic	Dynamic	Dynamic
Cartesian (Kleinman Symm)	33.6	42.2	NaN +/- NaN	NaN
Mixed-Spherical (Kleinman Symm)	33.7	42.2	NaN +/- NaN	NaN

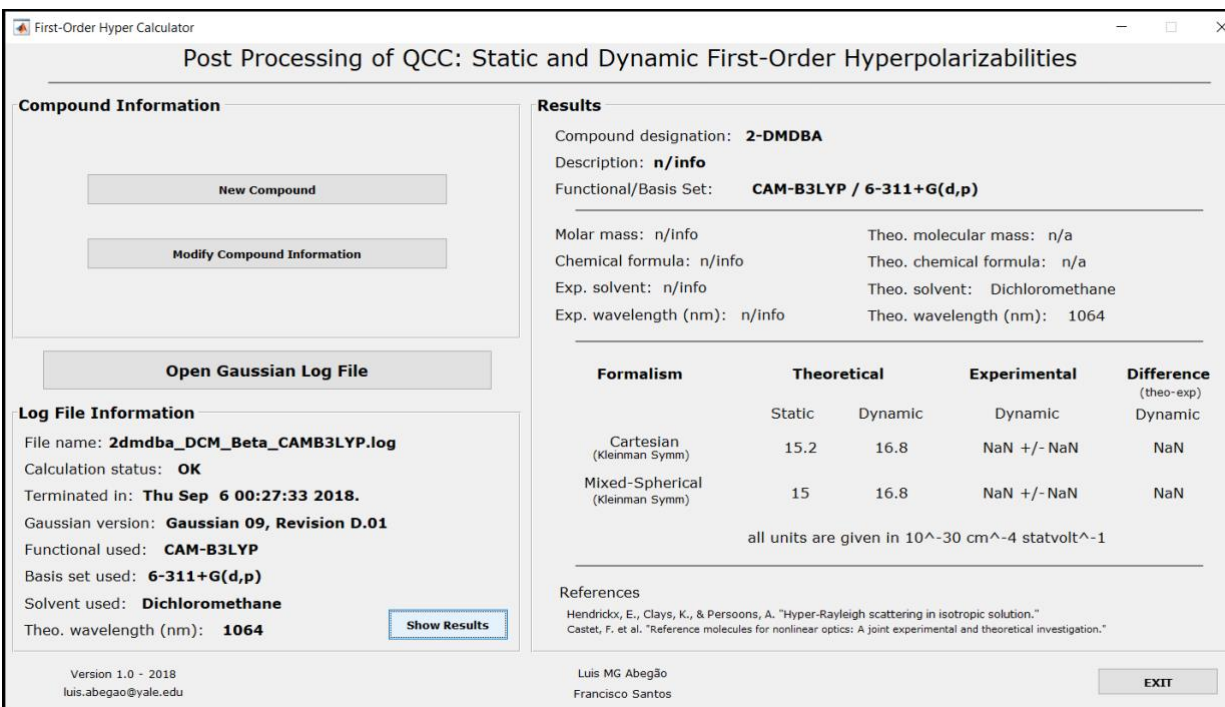
all units are given in 10⁻³⁰ cm⁻⁴ statvolt⁻¹

References

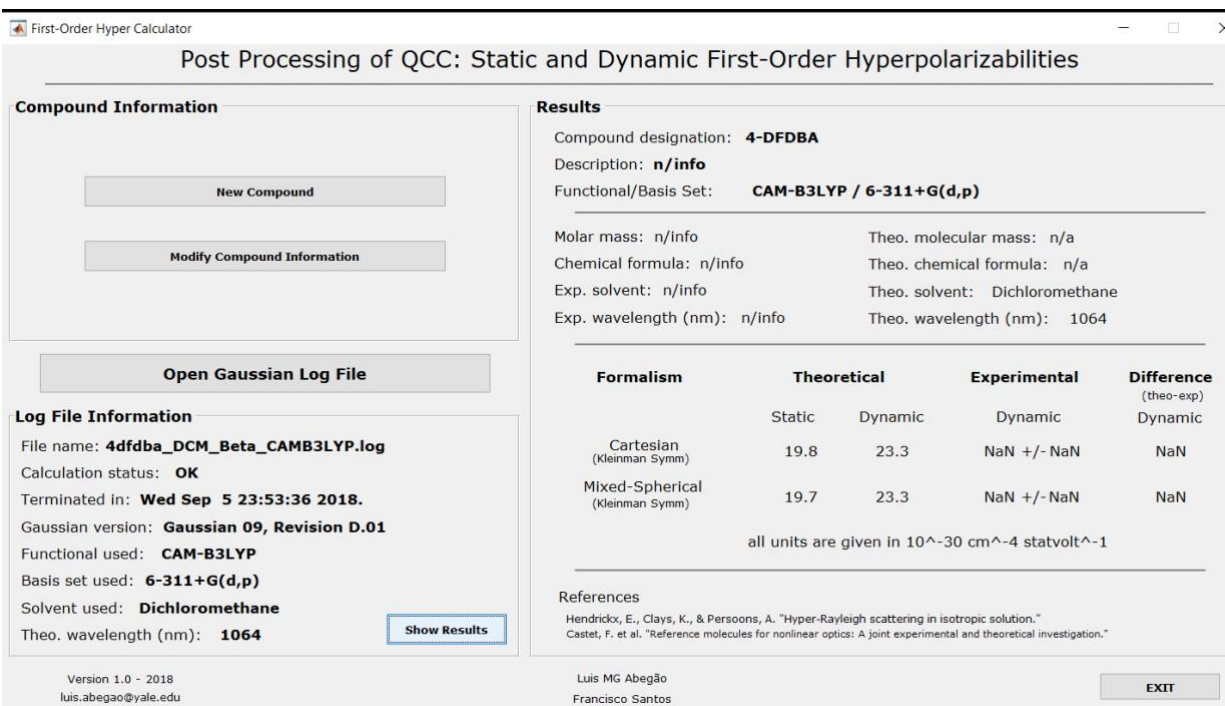
Hendrickx, E., Clays, K., & Persoons, A. "Hyper-Rayleigh scattering in isotropic solution."
 Castet, F. et al. "Reference molecules for nonlinear optics: A joint experimental and theoretical investigation."

Version 1.0 - 2018
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Francisco Santos
[EXIT](#)

Molecule: 4-DMDBA



Molecule: 2-DMDBA



Molecule: 4-DFDBA