

Supplementary Data

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

The screenshot displays the 'First-Order Hyper Calculator' software interface. The main window title is 'Post Processing of QCC: Static and Dynamic First-Order Hyperpolarizabilities'. The interface is divided into several sections:

- Compound Information:** Contains buttons for 'New Compound' and 'Modify Compound Information'.
- Log File Information:** Displays file name 'C3_DCM_Beta_CAMB3LYP.log', calculation status 'OK', termination time 'Sun Sep 9 21:33:49 2018', Gaussian version 'Gaussian 09, Revision D.01', functional 'CAM-B3LYP', basis set '6-311+G(d,p)', solvent 'Dichloromethane', and theoretical wavelength '1064'. A 'Show Results' button is present.
- Open Gaussian Log File:** A button to open the log file.
- Results:** Shows compound designation 'Chalcone C-3', description 'n/info', and functional/basis set 'CAM-B3LYP / 6-311+G(d,p)'. It lists molar mass, chemical formula, solvent, and wavelength for both experimental and theoretical values.
- Table:** A table comparing formalisms (Cartesian and Mixed-Spherical) with theoretical and experimental static and dynamic hyperpolarizabilities. Theoretical values are 14.5 and 14.4, while experimental values are NaN +/- NaN. The difference is also NaN.
- References:** Lists two references: Hendrickx, E., Clays, K., & Persoons, A. (2004) and Castet, F. et al. (2004).
- Footer:** Includes version '1.0 - 2018', contact 'luis.abegao@yale.edu', and authors 'Luis MG Abegão' and 'Francisco Santos'. An 'EXIT' button is also present.

Molecule: C-3

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: **C4_DCM_Beta_CAMB3LYP.log**
 Calculation status: **OK**
 Terminated in: **Sun Sep 9 21:48:49 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: **Chalcone C-4**
 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
	Static	Dynamic	Dynamic	(theo-exp)
Cartesian (Kleinman Symm)	26.6	35	NaN +/- NaN	NaN
Mixed-Spherical (Kleinman Symm)	26.6	35	NaN +/- NaN	NaN

all units are given in $10^{-30} \text{ cm}^{-4} \text{ statvolt}^{-1}$

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."

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Version 1.0 - 2018
luis.abegao@yale.edu
Luis MG Abegão
Francisco Santos

Molecule: C-4

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: **C5_DCM_Beta_CAMB3LYP.log**
 Calculation status: **OK**
 Terminated in: **Thu Oct 25 21:01:09 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: **Chalcone C-5**
 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
	Static	Dynamic	Dynamic	(theo-exp)
Cartesian (Kleinman Symm)	27.3	35.4	NaN +/- NaN	NaN
Mixed-Spherical (Kleinman Symm)	27.4	35.4	NaN +/- NaN	NaN

all units are given in $10^{-30} \text{ cm}^{-4} \text{ statvolt}^{-1}$

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."

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Version 1.0 - 2018
luis.abegao@yale.edu
Luis MG Abegão
Francisco Santos

Molecule: C-5

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: **C6_DCM_Beta_CAMB3LYP.log**
 Calculation status: **OK**
 Terminated in: **Sun Sep 9 22:24:42 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: **Chalcone C-6**
 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
	Static	Dynamic	Dynamic	(theo-exp)
Cartesian (Kleinman Symm)	13.9	21.9	NaN +/- NaN	NaN
Mixed-Spherical (Kleinman Symm)	13.8	21.9	NaN +/- NaN	NaN

all units are given in $10^{-30} \text{ cm}^{-4} \text{ statvolt}^{-1}$

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."

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Version 1.0 - 2018
luis.abegao@yale.edu

Luis MG Abegão
Francisco Santos

Molecule: C-6

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: **C7_DCM_Beta_CAMB3LYP.log**
 Calculation status: **OK**
 Terminated in: **Sun Sep 9 22:47:44 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: **Chalcone C-7**
 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
	Static	Dynamic	Dynamic	(theo-exp)
Cartesian (Kleinman Symm)	15.8	19.1	NaN +/- NaN	NaN
Mixed-Spherical (Kleinman Symm)	15.8	19.1	NaN +/- NaN	NaN

all units are given in $10^{-30} \text{ cm}^{-4} \text{ statvolt}^{-1}$

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."

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luis.abegao@yale.edu

Luis MG Abegão
Francisco Santos

Molecule: C-7