Data for Cyclopropyl substituents transform the viscosity-sensitive BODIPY molecular rotor into a temperature sensor, in ACS Sensors

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DFT and linear response time-dependent DFT (TDDFT) calculations were carried out, with the Gaussian 09 code.[1] The files are organised by molecule: BODIPY-C10, BODIPY-2 and BODIPY-3. Within each molecule folder there three folders:

- Ground state calculations 'Ground'
- TDDFT calculations of the 1st vertically excited state 'Vertical'
- TDDFT geometry optimisations on the 1st adiabatically relaxed excited state 'Adiabatic'

Each folder contains the Gaussian log files, which have the extension *.log. Calculations that have been restarted are saved with two files: *old.log - the initial calculation and *.log - the final calculation. Each Gaussian log file, at the start contains a written copy of the input file used to create it. Input files have the extension *.in. The system for naming input files is as follows:

- Numerical numbers represent the value that the phenyl ring dihedral angle, in degrees, which was constrained to during the simulation e.g. 80.in represents a calculation where the torsional angle was constrained to 80°
- 'Uncons' refers to an unconstrained simulations, where no constraints were applied to any atom

References

[1] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F.

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