



**Jens Spanget-Larsen (emer.):
Computerkemi og Molekylspektroskopi
Udvalgte resultater 2017-2021**

October 06, 2021
Institut for Naturvidenskab og Miljø
Roskilde Universitet (RUC)

Eksempler på forskning og publikationsvirksomhed

- (1) Samarbejde med Danijela Bakaric (née Vojta)
- (2) Jod og pyridin i polyethylen (Huong Thu Nguyen)
- (3) 'Synchrotron Radiation Linear Dichroism' (SRLD)
UV spektroskopi
- (4) 'Electron Spin Resonance' (ESR, EPR)
spektroskopi



Danijela Bakaric, née Vojta

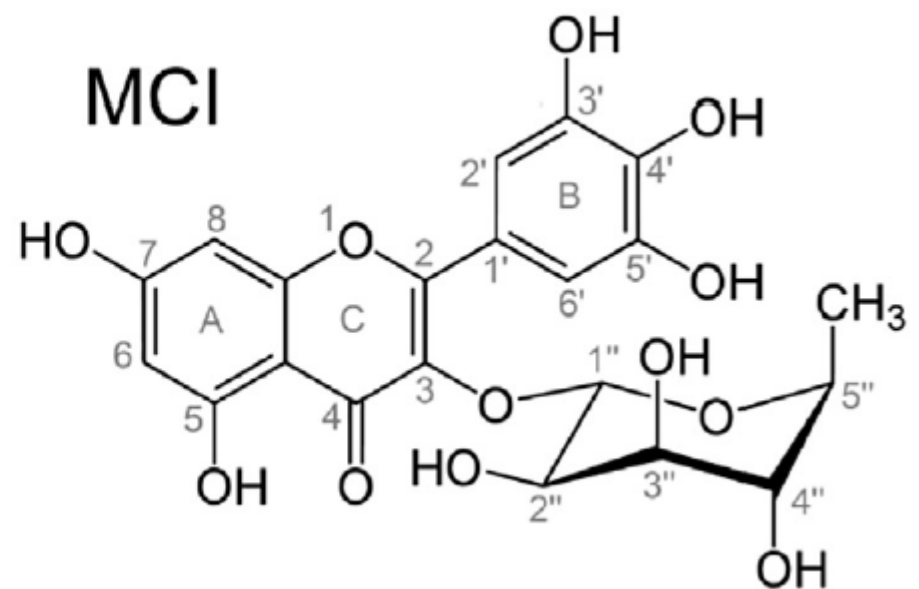
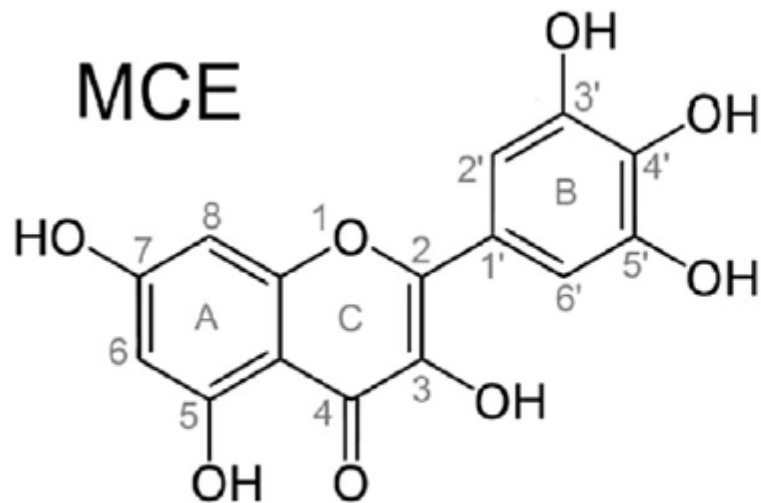
Electronic states of Myricetin. UV-Vis polarization spectroscopy and quantum chemical calculations☆

Danijela Vojta ^{a,*}, Eva Marie Karlsen ^b, Jens Spanget-Larsen ^{b,*}

(2017)

Intramolecular hydrogen bonding in myricetin and myricitrin. Quantum chemical calculations and vibrational spectroscopy

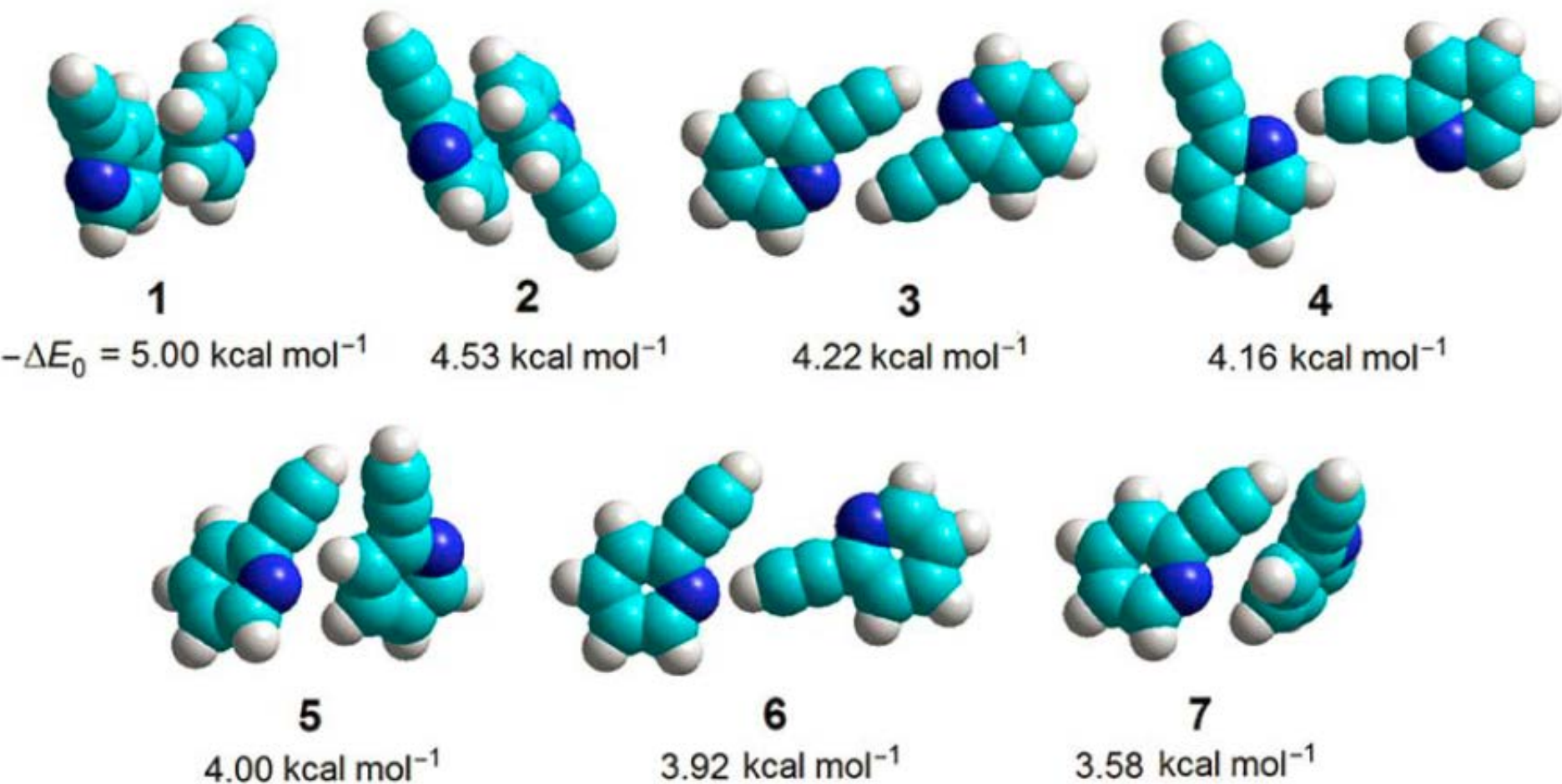
Danijela Vojta ^{a,*}, Katarina Dominković ^b, Snežana Miljanić ^c, Jens Spanget-Larsen ^{d,**}



2-Ethynylpyridine dimers: IR spectroscopic and computational study

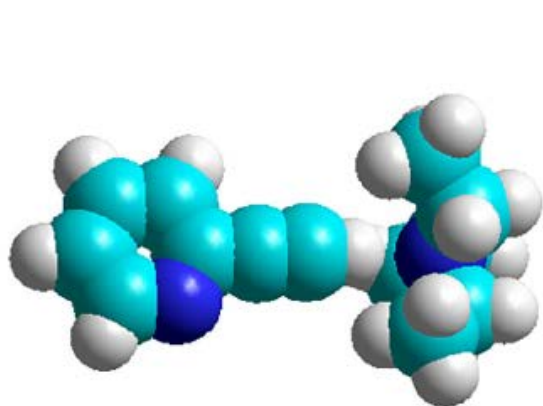
Danijela Bakarić^{a,*}, Jens Spanget-Larsen^{b,*}

(2018)

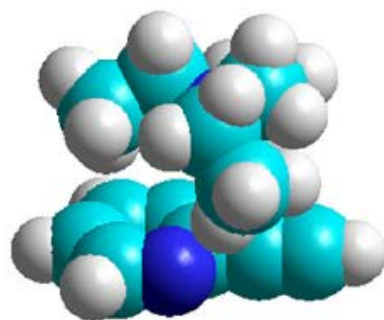


Hydrogen bonding between ethynyl aromates and triethylamine: IR spectroscopic and computational study (2019)

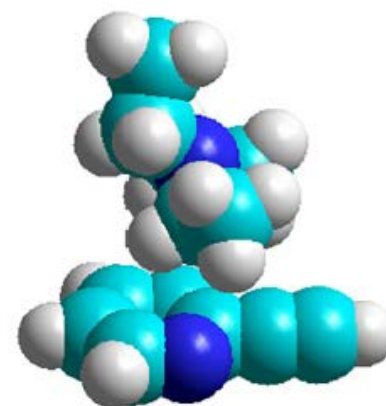
Danijela Bakarić ^{a,*}, Josipa Alerić ^b, Tijana Parlić-Risović ^b, Jens Spanget-Larsen ^{c,*}



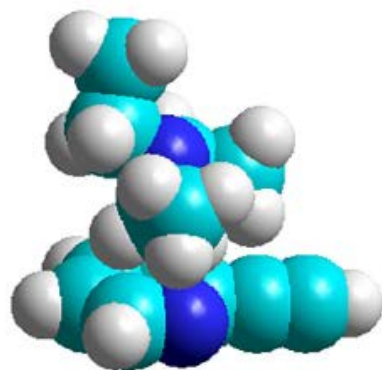
$$-\Delta E_0 = 4.57 \text{ kcal mol}^{-1}$$



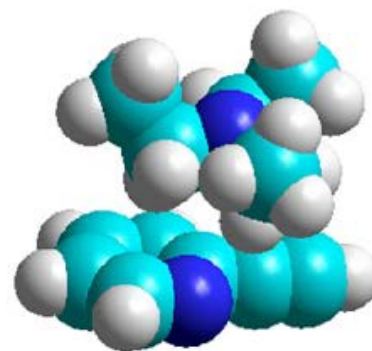
$$3.79 \text{ kcal mol}^{-1}$$



$$3.56 \text{ kcal mol}^{-1}$$



$$3.38 \text{ kcal mol}^{-1}$$



$$3.27 \text{ kcal mol}^{-1}$$

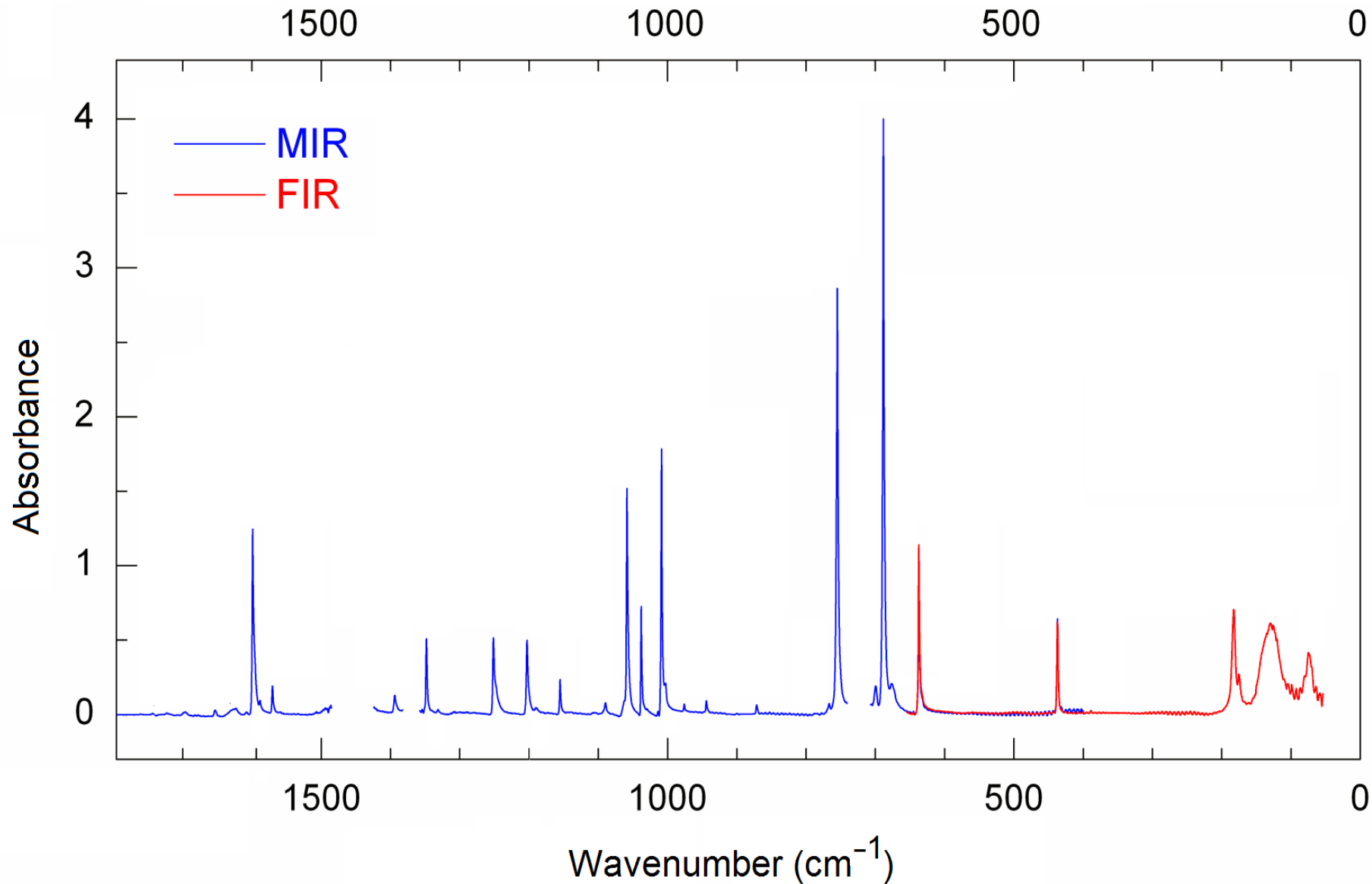


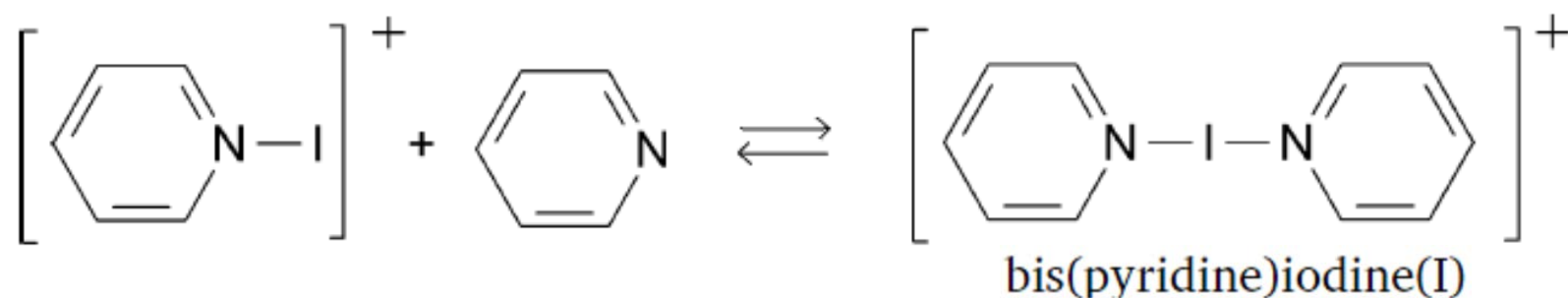
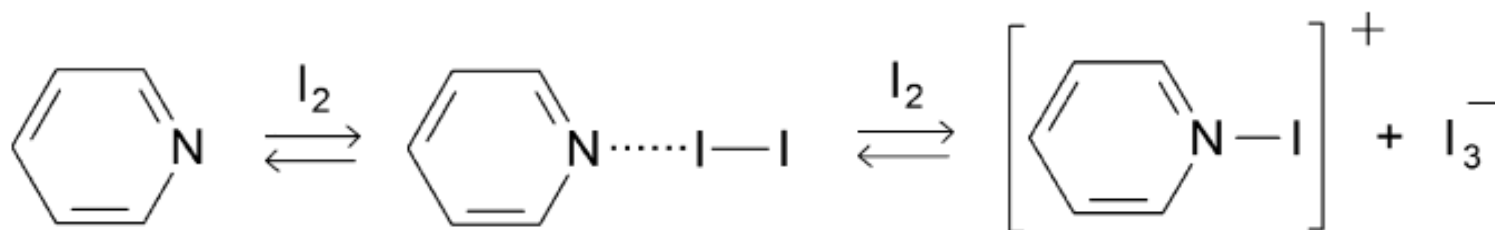
Huong Thu Nguyen
(photo from 2009)



Pyridine + Iodine

Pyridine + iodine in stretched PE
after evaporation of volatile substances



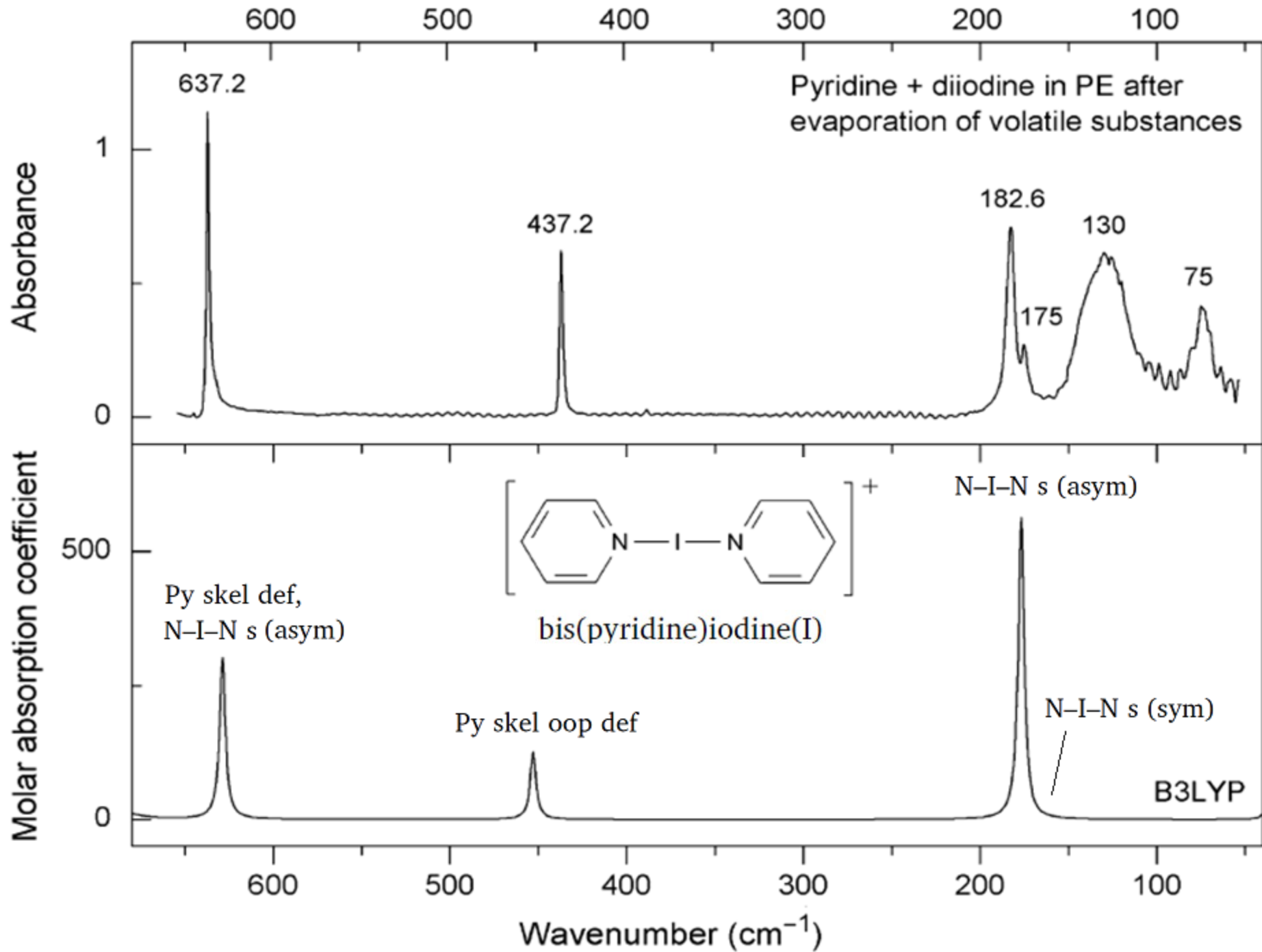


Ionic reaction products of iodine with pyridine, 4-methylpyridine, and 4-*tert*-butylpyridine in a polyethylene matrix. A FTIR polarization spectroscopic investigation

(2019)

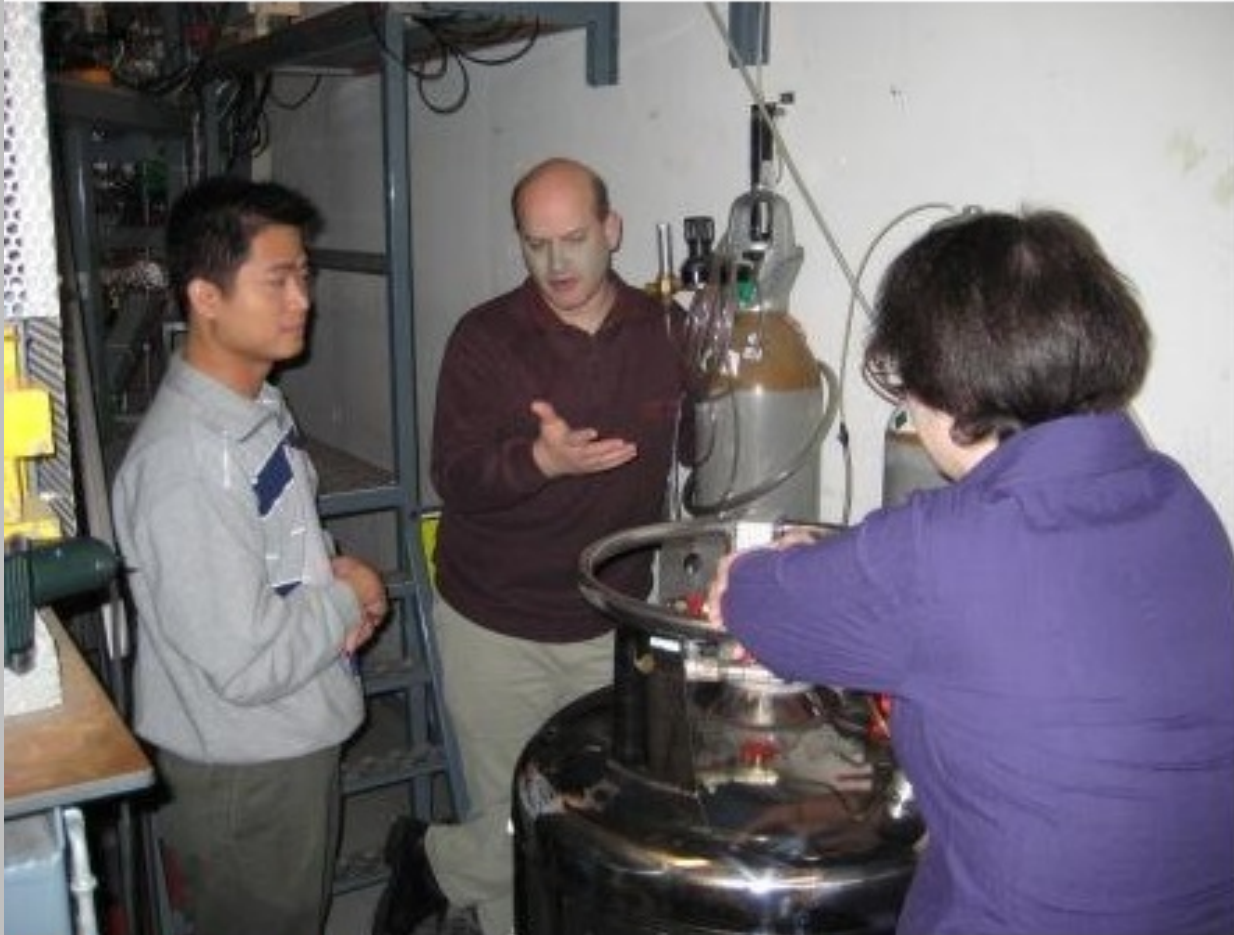
Huong Thu Nguyen¹, Duy Duc Nguyen², Jens Spanget-Larsen*

In spite of their elongated molecular shape, the bis(pyridine)iodine(I) and bis(4-methylpyridine)iodine(I) cations are randomly aligned in stretched polyethylene; they probably form micro-crystalline polyiodide aggregates in the amorphous regions of the polymer.



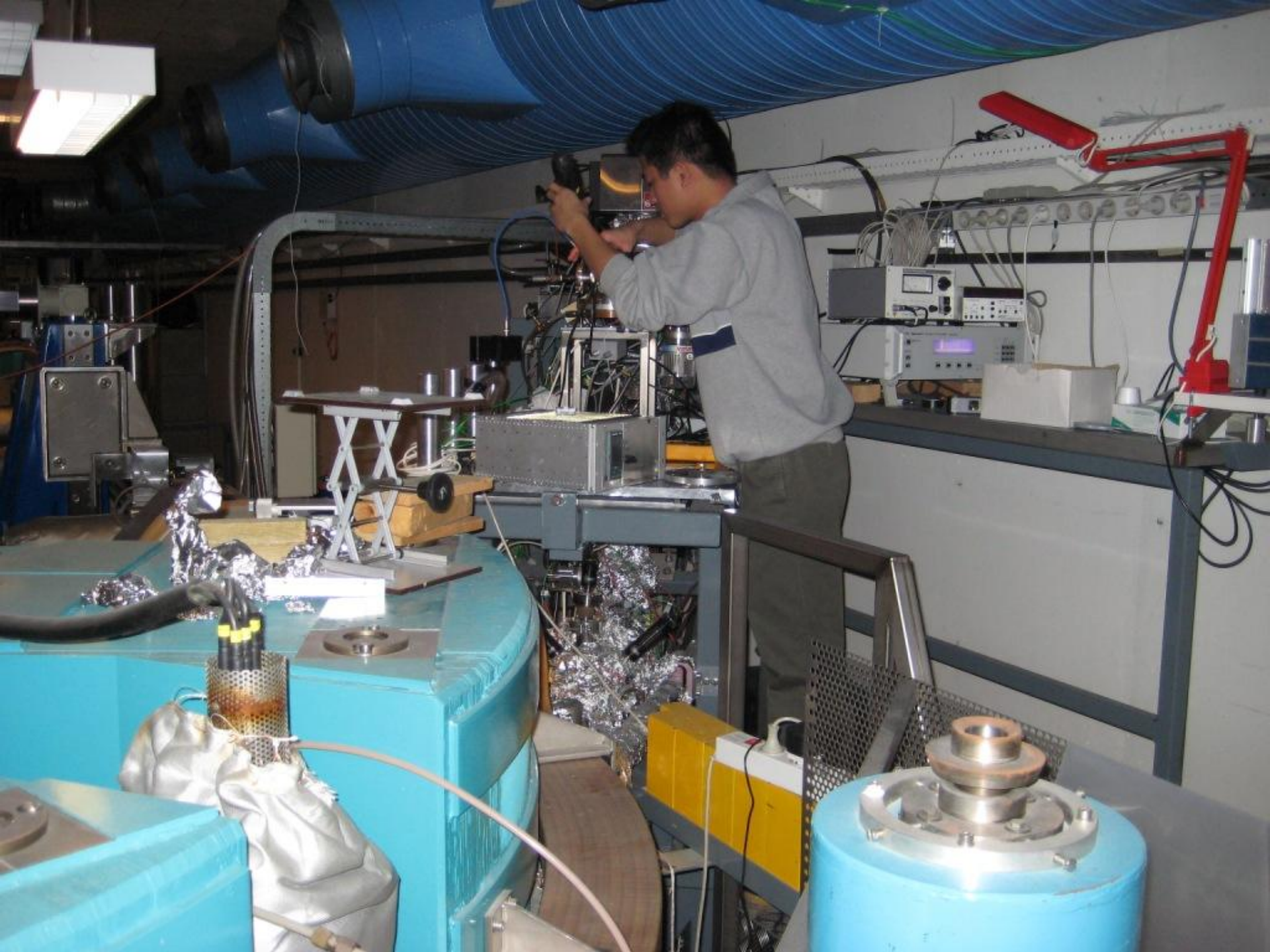
Synchrotron Radiation Linear Dichroism (SRLD) Spectroscopy at ISA, Aarhus University

Søren Vrønning Hoffmann




Duy Duc Nguyen

Nykola C. Jones



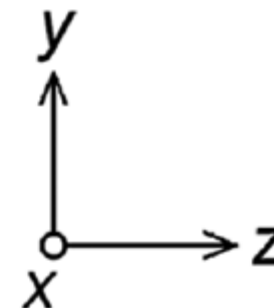
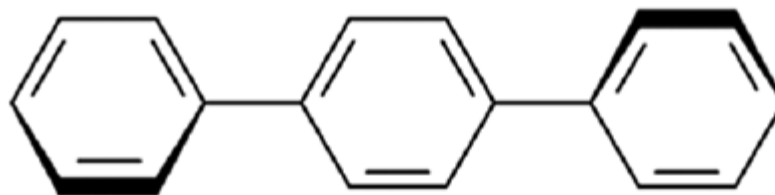
Vacuum UV Polarization Spectroscopy of *p*-Terphenyl (2018)

Duy Duc Nguyen,^{†,#} Nykola C. Jones,[‡] Søren V. Hoffmann,[‡] and Jens Spanget-Larsen^{*,†} 

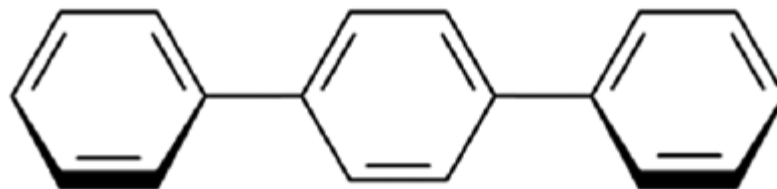
[†]Department of Science and Environment, Roskilde University, Universitetsvej 1, DK-4000 Roskilde, Denmark

[‡]ISA, Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, Bldg. 1520, DK-8000 Aarhus C, Denmark

D_2

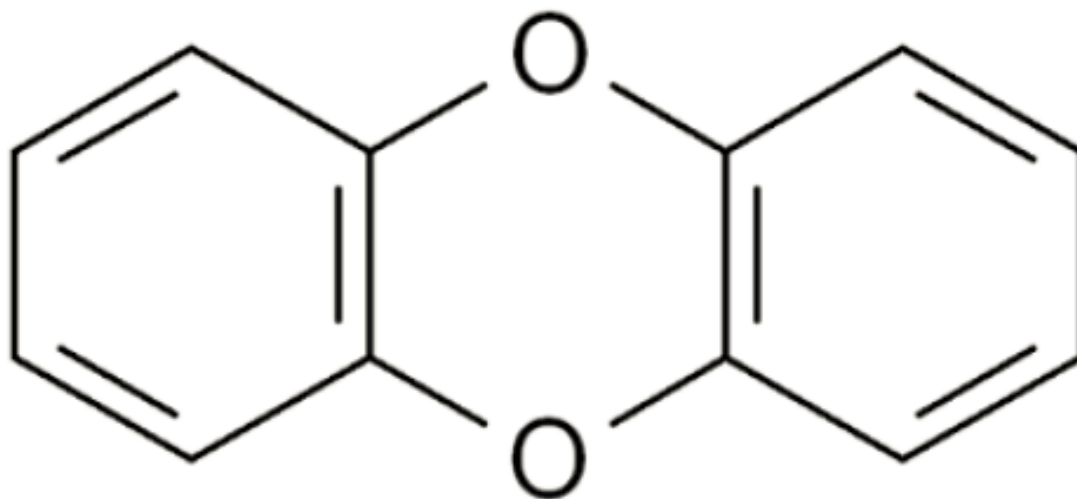


C_{2h}



Electronic states of dibenzo-*p*-dioxin. A synchrotron radiation
linear dichroism investigation (2019)

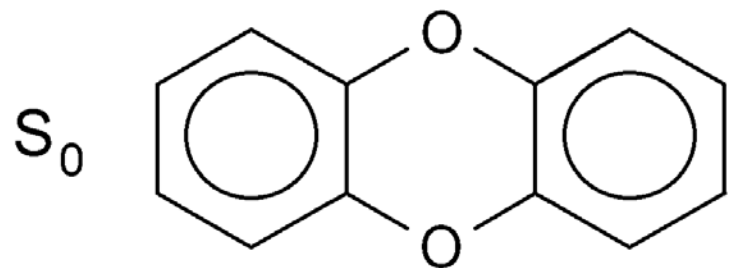
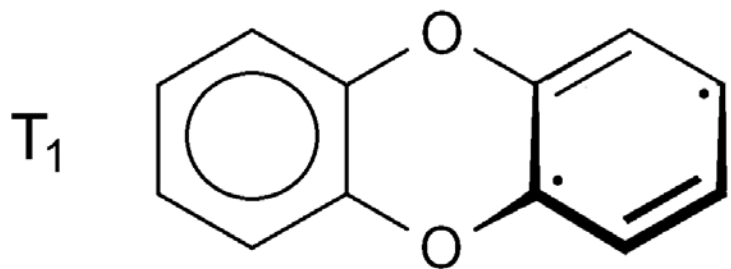
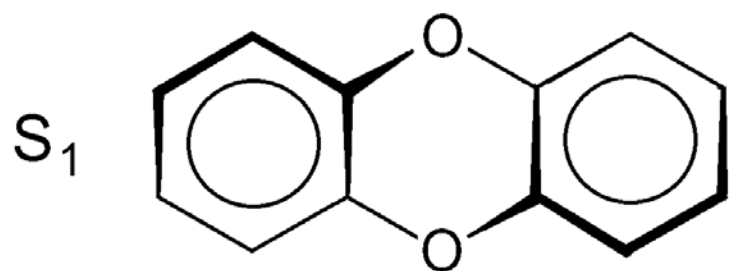
Duy Duc Nguyen^{a,1}, Nykola C. Jones^b, Søren V. Hoffmann^b, Jens Spanget-Larsen^{a,*}



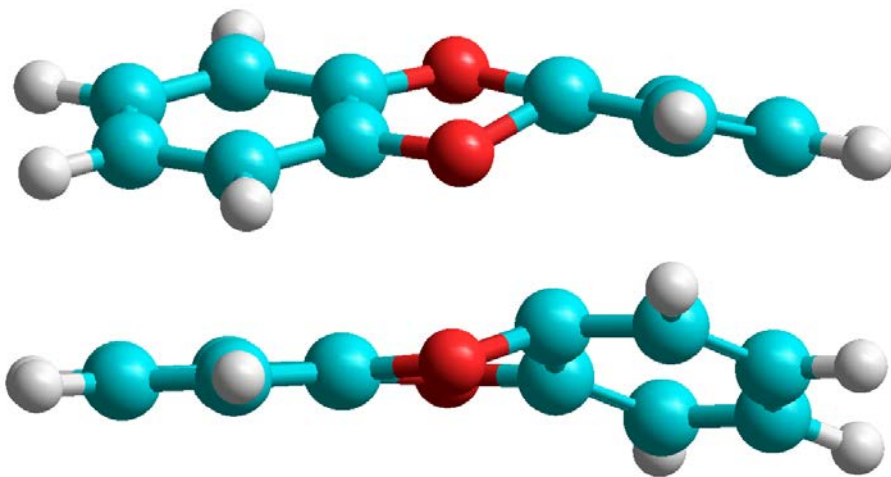
Dibenzo-*p*-dioxin. Twisted and puckered excited state molecular geometries

Jens Spanget-Larsen

(2019)

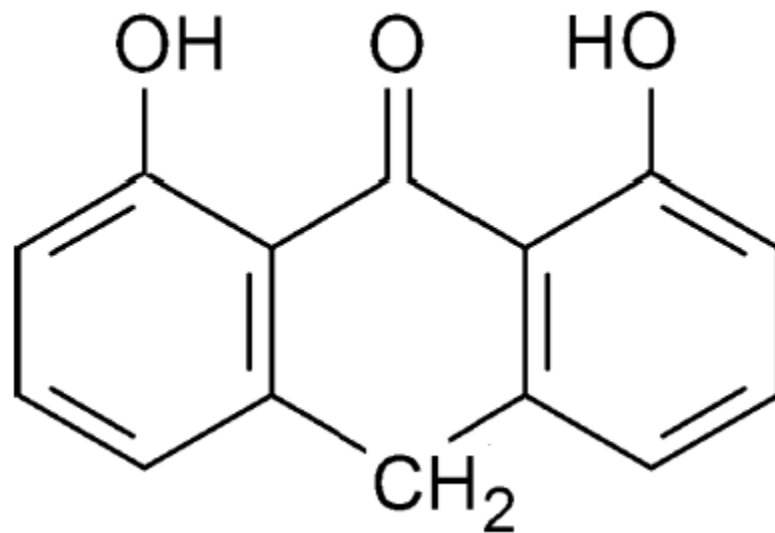


Triplet state, T_1

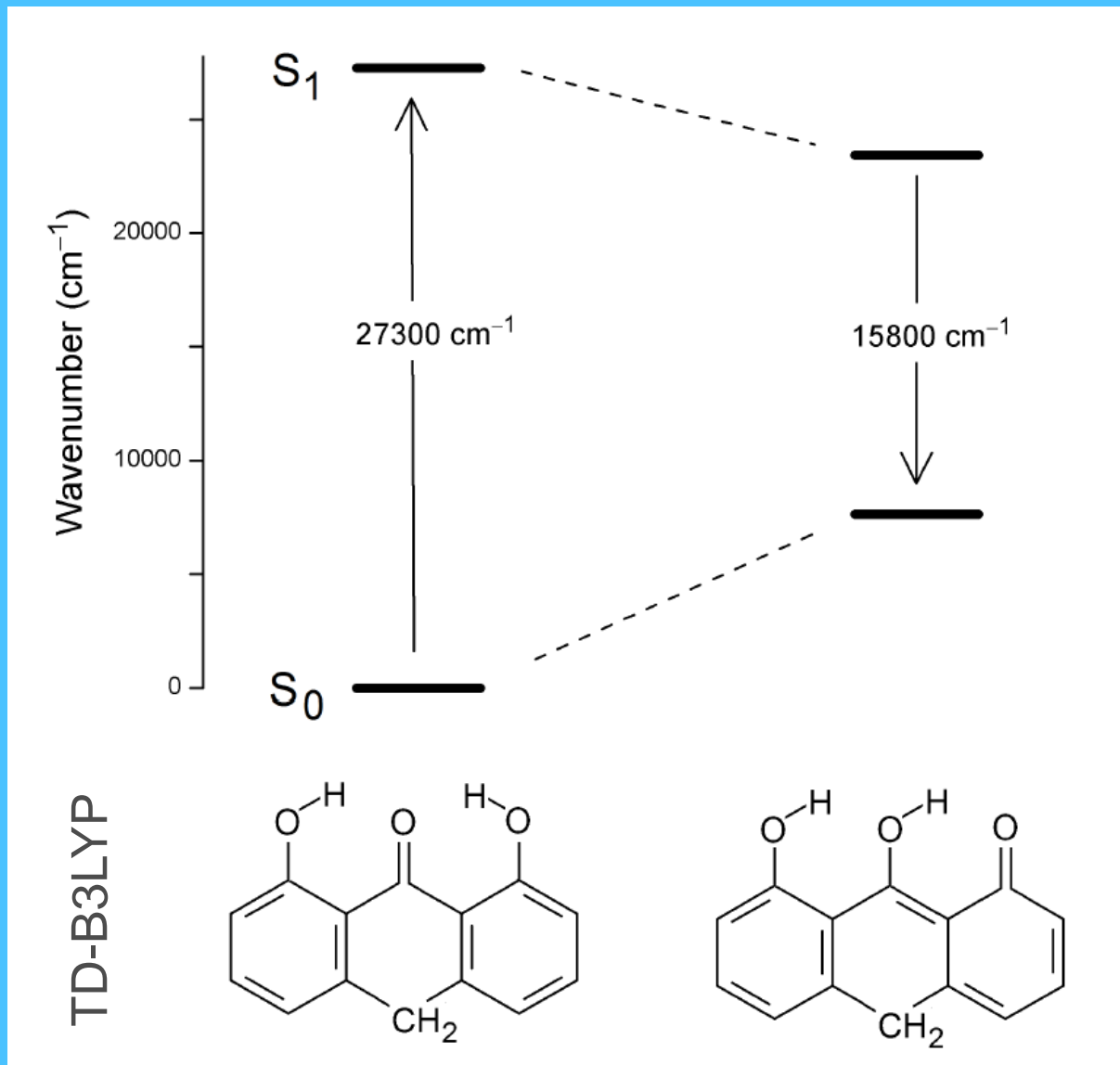


UV synchrotron radiation linear dichroism spectroscopy of the anti-psoriatic drug anthralin (2019)

Duy Duc Nguyen^{1,3}, Nykola C. Jones², Søren Vrønning Hoffmann² and Jens Spanget-Larsen¹



Excited State Intramolecular Proton Transfer (ESIPT)





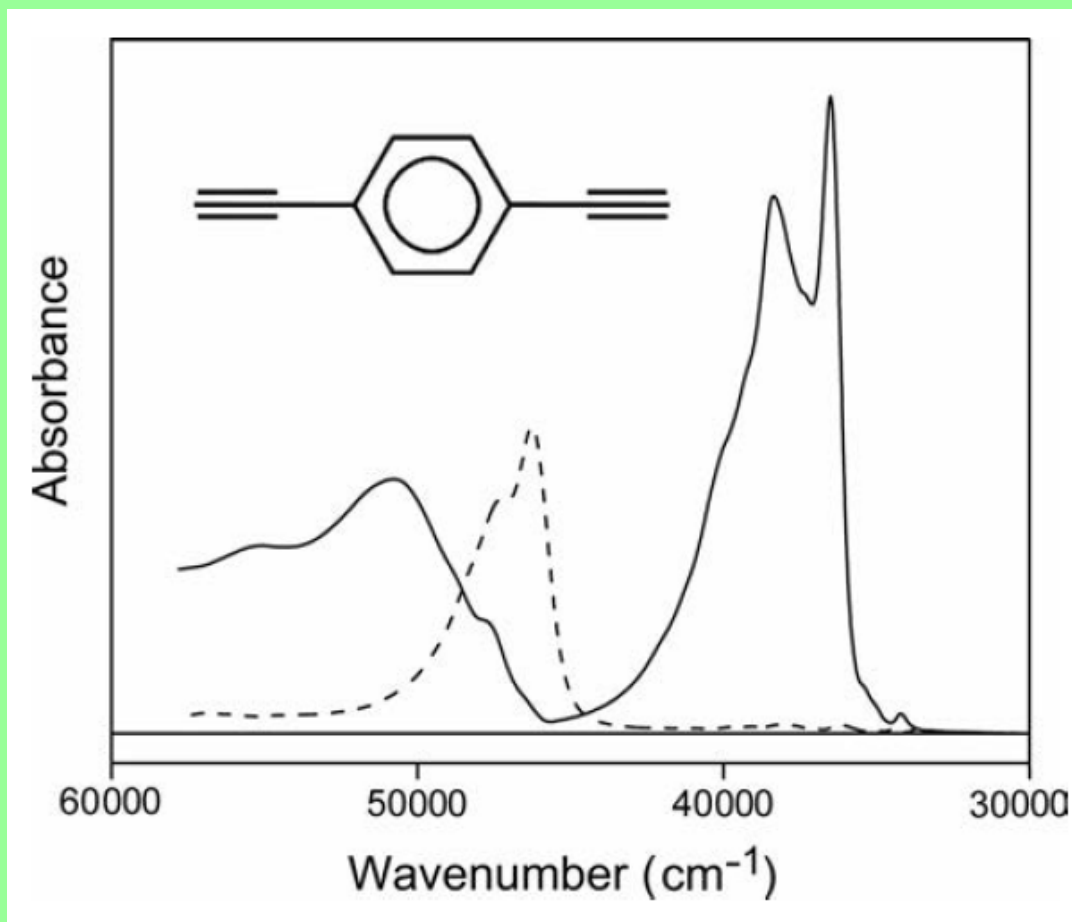
Peter W. Thulstrup klargør en prøve til LD-spektroskopi med cyklotron-stråling ved ISA, Centre for Storage Ring Facilities, Aarhus Universitet.



UV polarisation spectroscopy of 1,4-diethynylbenzene

(2021)

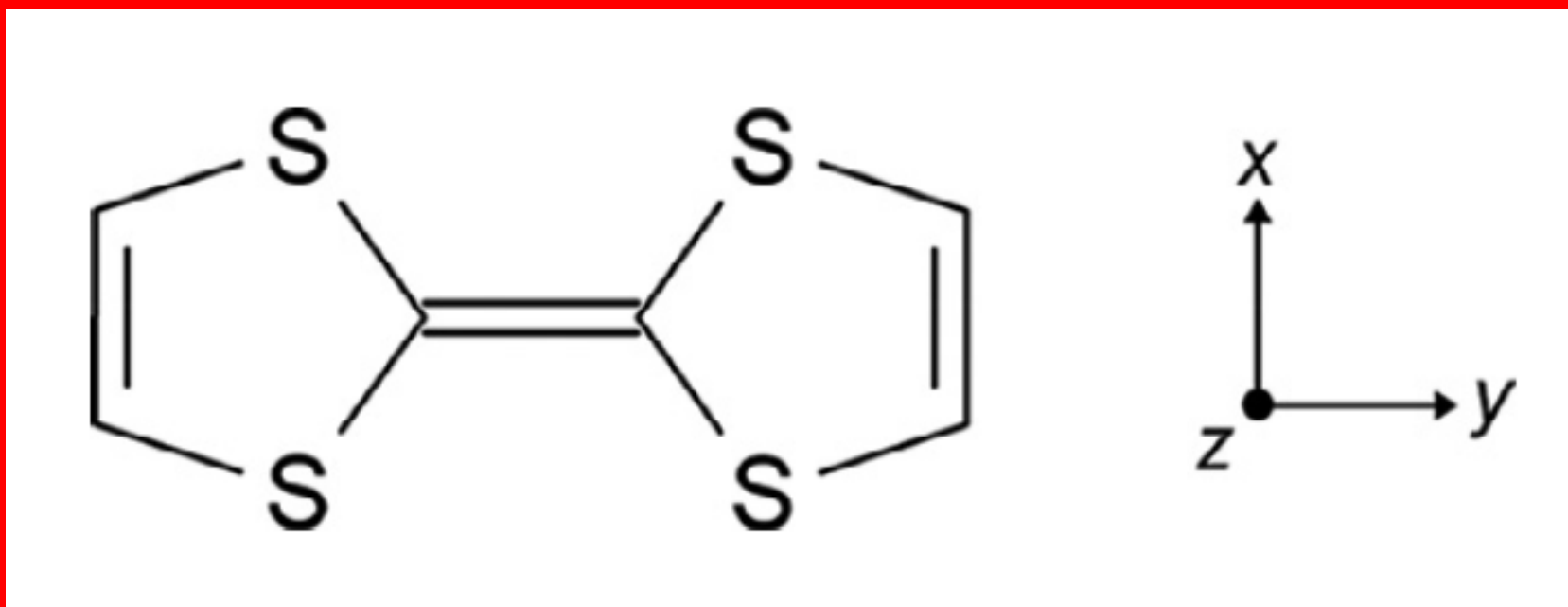
Peter W. Thulstrup, Nykola C. Jones, Søren V. Hoffmann & Jens Spanget-Larsen



Electronic transitions of tetrathiafulvalene oriented in polyethylene film. Near and vacuum UV synchrotron radiation polarization spectroscopy

P.W. Thulstrup^{a,*}, S.V. Hoffmann^b, N.C. Jones^b, J. Spanget-Larsen^{c,*}

(2021)

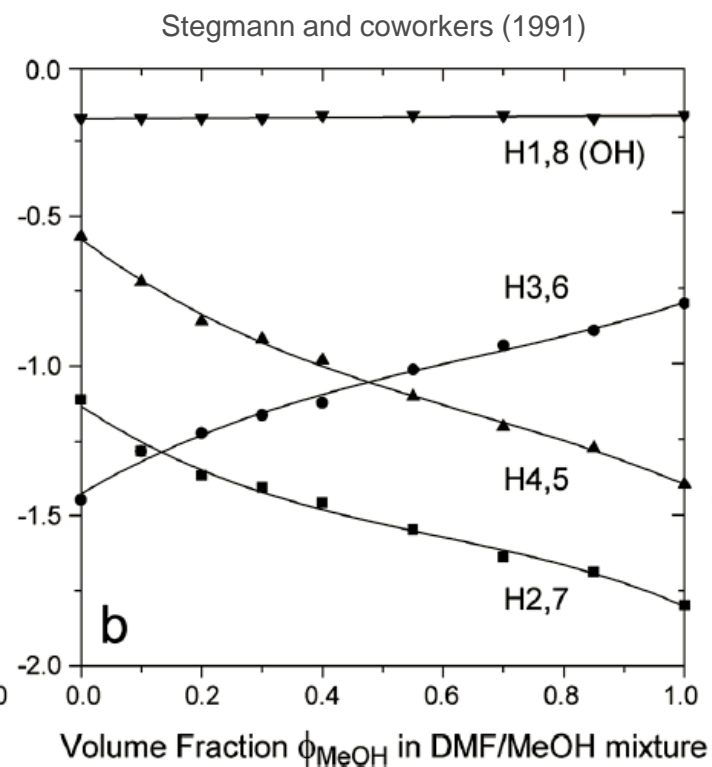
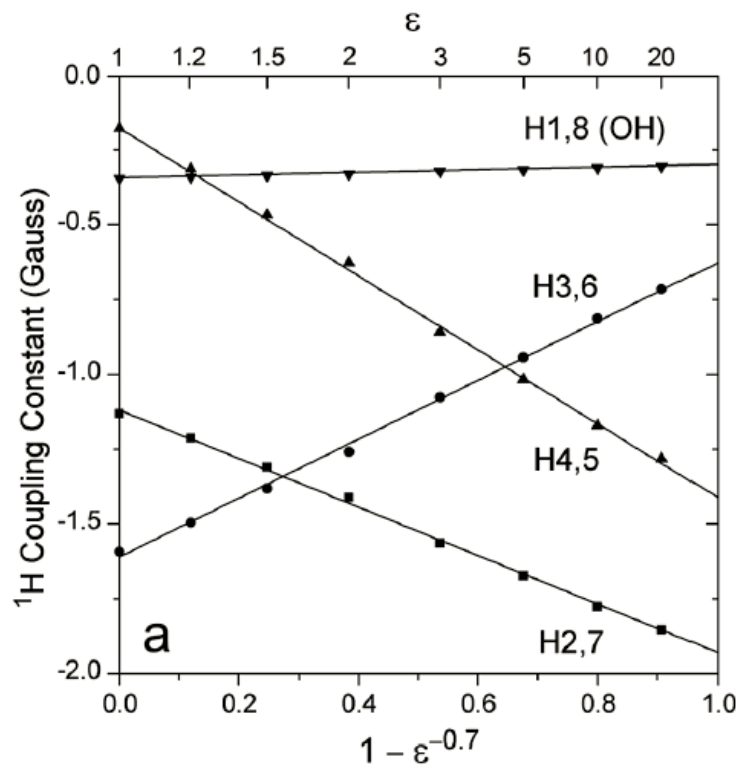
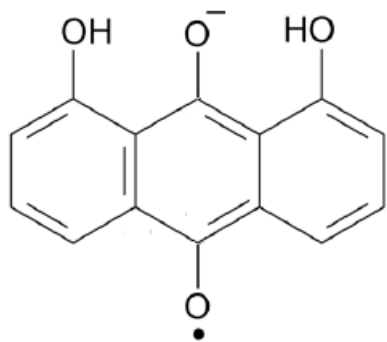


Electron Spin Resonance (ESR, EPR) Spectroscopy

Chryszazin semiquinone radical anion. A theoretical study of the influence of the solvent on the electron spin resonance spectrum

(2020)

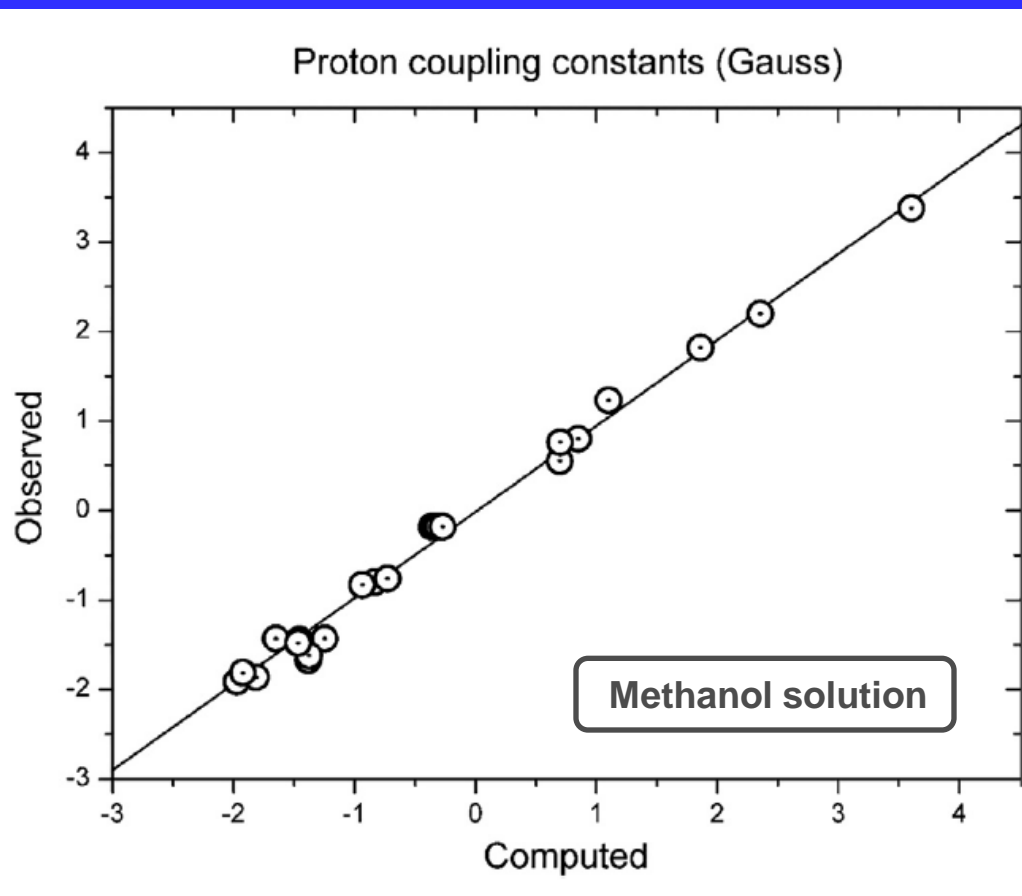
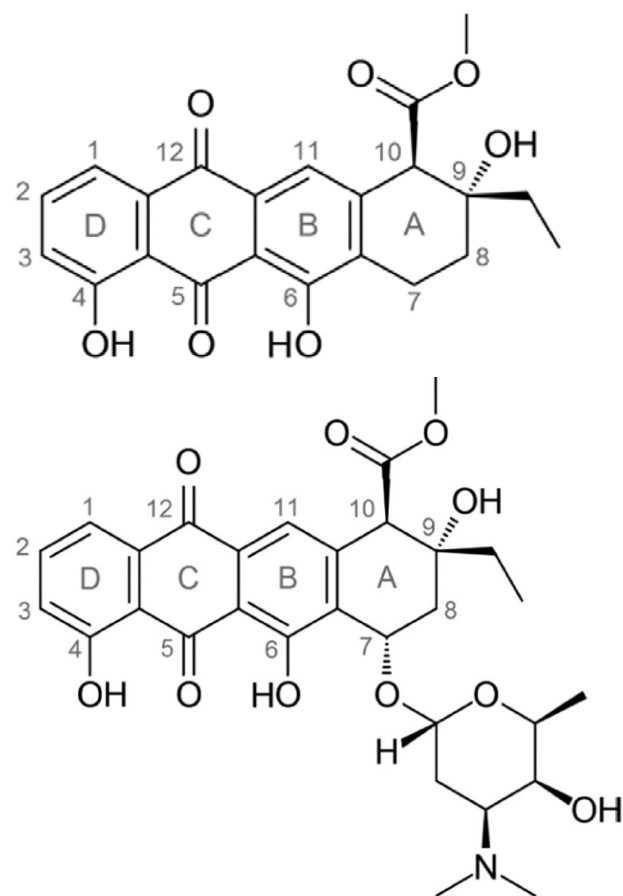
Jens Spanget-Larsen



Semiquinone radical anions derived from 2,3-dimethylchrysin, 7-deoxyaklavinone, and aclacinomycin T. Computational studies of the influence of aprotic and protic solvents on the electron spin resonance spectra

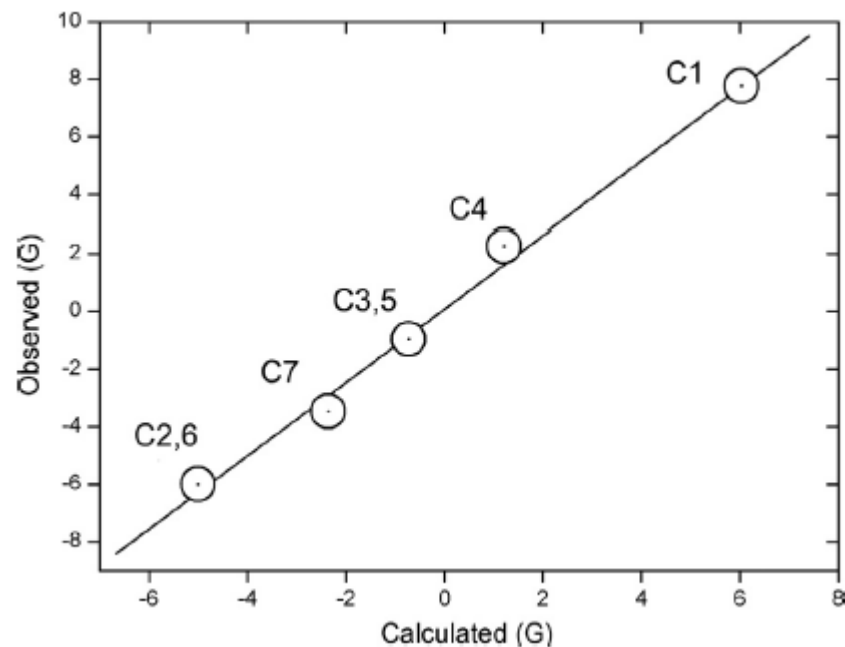
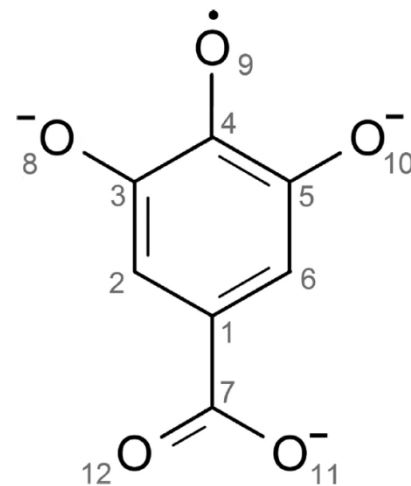
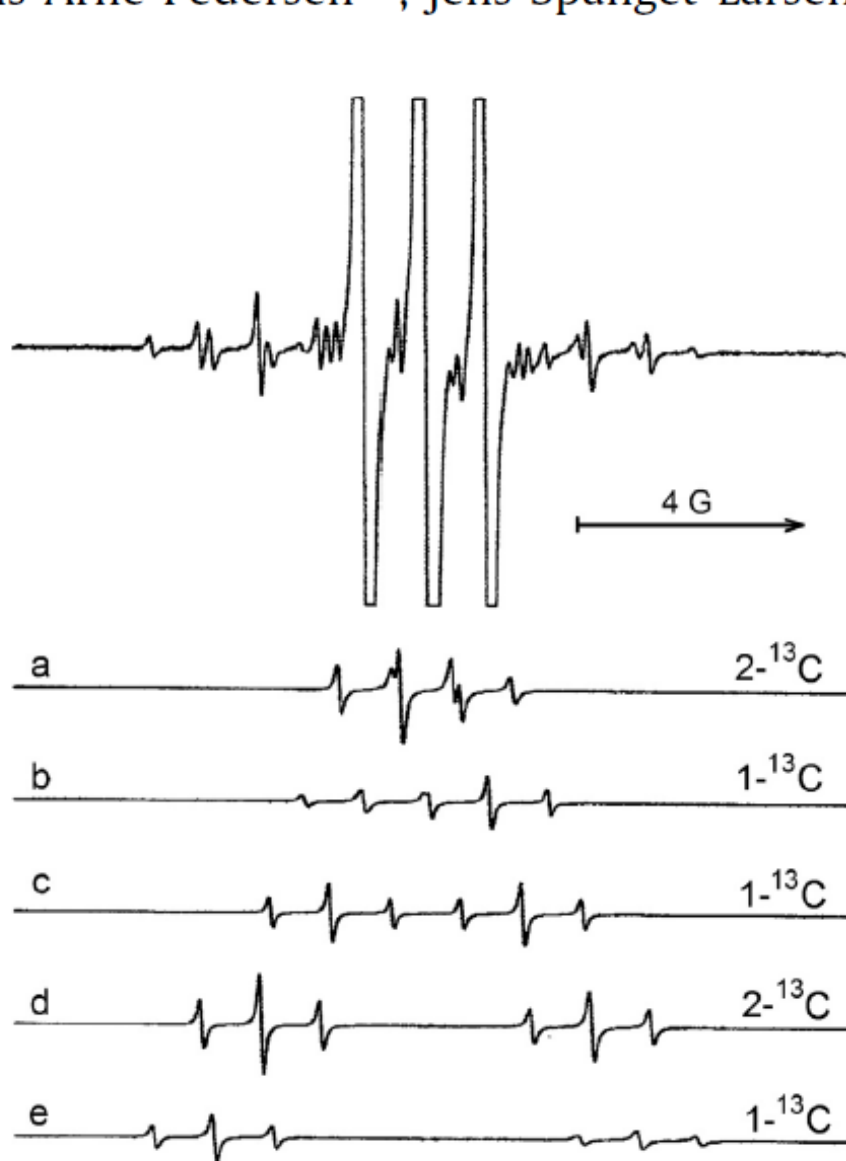
Jens Spanget-Larsen

(2020)



Gallate semiquinone radical tri-anion. Experimental and theoretical studies of the ^{13}C hyperfine coupling constants (2021)

Jens Arne Pedersen^{a,§}, Jens Spanget-Larsen^{b,*}





Publications 2017-2021

1. D. Vojta, E. M. Karlsen, J. Spanget-Larsen: “Electronic states of myricetin. UV-Vis polarization spectroscopy and quantum chemical calculations”, *Spectrochim. Acta A* **173**, 182-187 (2017).
2. D. Vojta, K. Dominković, S. Miljanić, J. Spanget-Larsen: “Intramolecular hydrogen bonding in myricetin and myricitrin. Quantum chemical calculations and vibrational spectroscopy”, *J. Mol. Struct.* **1131**, 242-249 (2017).
3. P. E. Hansen, J. Spanget-Larsen: “Review: NMR and IR investigations of strong intramolecular hydrogen bonds”, *Molecules* **22**, 552, pp 1-21 (2017). Open Access: <http://dx.doi.org/10.3390/molecules22040552>.
4. E. W. Thulstrup, J. Spanget-Larsen: “Spektroskopi med lineært polariseret lys”, *Molekylspektroskopi – et stykke dansk kemihistorie*, Historisk-kemiske skrifter nr. 23, udgivet af Dansk Selskab for Historisk Kemi & Dansk Forening for Molekylspektroskopi, Kapitel 7, pp155-175 (November 2017).
5. D. Bakarić, J. Spanget-Larsen: “2-Ethynylpyridine dimers: IR spectroscopic and computational study”, *Spectrochim. Acta A* **195**, 41-46 (2018).
6. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “Vacuum UV Polarization Spectroscopy of *p*-Terphenyl”, *J. Phys. Chem. A* **122**, 184-191 (2018).
7. D. Bakarić, J. Alerić, T. Parlić-Risović, J. Spanget-Larsen: “Hydrogen bonding between ethynyl aromates and triethylamine: IR spectroscopic and computational study”, *Spectrochim. Acta A* **209**, 288-294 (2019).

8. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “Electronic states of dibenzo-*p*-dioxin. A synchrotron radiation linear dichroism investigation”, *Chem. Phys.* **519**, 64-68 (2019).
9. H. T. Nguyen, D. D. Nguyen, J. Spanget-Larsen: “Ionic reaction products of iodine with pyridine, 4-methylpyridine, and 4-*tert*-butylpyridine in a polyethylene matrix. A FTIR polarization spectroscopic investigation”, *Chem. Phys. Lett.* **62**, 1004-1015 (2019).
10. P. E. Hansen, A. Jezierska, J. Panek, J. Spanget-Larsen: “Theoretical Calculations Are a Strong Tool in the Investigation of Strong Intramolecular Hydrogen Bonds”, in *Molecular Spectroscopy: A Quantum Chemistry Approach*, Y. Ozaki, M. J. Wójcik, J. Popp (Eds.), Volume 1, Chapter 8, pp 215-251; Wiley-VCH, Weinheim 2019.
11. J. Spanget-Larsen, “Dibenzo-*p*-dioxin. Twisted and puckered excited state molecular geometries”, *Comput. Theor. Chem.* **1164**, 112551, pp 1-4 (2019).
12. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “UV synchrotron radiation linear dichroism investigation of the anti-psoriatic drug anthralin”, *PeerJ Physical Chemistry* **1**:e5, pp 1-14 (2019). Open Access: <https://doi.org/10.7717/peerj-pchem.5>.
13. P. E. Hansen, F. S. Kamounah, B. A. Saeed, M. J. MacLachlan, J. Spanget-Larsen: “Intramolecular Hydrogen Bonds in Normal and Sterically Compressed *o*-Hydroxy Aromatic Aldehydes. Isotope Effects on Chemical Shifts and Hydrogen Bond Strength”, *Molecules* **24**, 4533, pp 1-15 (2019). Open Access: <http://dx.doi.org/10.3390/molecules24244533>
14. J. Spanget-Larsen: “Chrysazin semiquinone radical anion. A theoretical study of the influence of the solvent on the electron spin resonance spectrum”, *Comput. Theor. Chem.* **1185**, 112878, pp 1-5 (2020).

15. J. Spanget-Larsen: “Semiquinone radical anions derived from 2,3-dimethylchrysin, 7-deoxyaklavinone, and aclacinomycin T. Computational studies of the influence of aprotic and protic solvents on the electron spin resonance spectra”, *J. Mol. Liquids* **320**, 114508, pp 1-7 (2020).
16. P. W. Thulstrup, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “UV polarization spectroscopy of 1,4-diethynylbenzene”, *Mol. Phys.* **119**, e1853841, pp 1-7 (2021). [dx.doi.org/10.1080/00268976.2020.1853841](https://doi.org/10.1080/00268976.2020.1853841).
17. P. W. Thulstrup, S. V. Hoffmann, N. C. Jones, J. Spanget-Larsen: “Electronic transitions of tetrathiafulvalene oriented in polyethylene film. Near and vacuum UV synchrotron radiation polarization spectroscopy”, *Chem. Phys. Impact* **2**, 100009, pp 1-6 (2021). Open Access: [dx.doi.org/10.1016/j.chphi.2020.100009](https://doi.org/10.1016/j.chphi.2020.100009).
18. J. A. Pedersen, J. Spanget-Larsen: “Gallate semiquinone radical tri-anion. Experimental and theoretical studies of the ^{13}C hyperfine coupling constants”, *J. Mol. Struct.* **1241**, 130663, pp 1-9 (2021). Open Access: [dx.doi.org/10.1016/j.molstruc.2021.130663](https://doi.org/10.1016/j.molstruc.2021.130663).

In preparation:

19. P. E. Hansen, M. Vakili, F. S. Kamounah, J. Spanget-Larsen: “NH stretching frequencies of intramolecularly hydrogen bonded systems. An experimental and theoretical study”.