



1a. Name:  1b. Title:   
2a. Department:  2b. Mailbox:   
3a. Email Address:  3b. Phone:   
4. Amount Requested:

5. Have You Received Funds from EDIT in the Last 2 Years?  Yes  No  
If Yes, Provide Details (Year / Cycle/ Amount):

6. Requested Funds from Other Sources:

A. Requested funds from Academic Affairs:  Yes  No  
Provide Details:   
B. Requested funds from Academic Department / Other:  Yes  No  
Provide Details:

7. Project Type (Choose One of the Following): Please note that the first 2 categories are for presentations at a conference or a Lecture while the 3<sup>rd</sup> and 4<sup>th</sup> categories are for conducting research in preparation for publication, etc. The 5<sup>th</sup> and 6<sup>th</sup> categories are for attending workshops, seminars, and conferences, not for presenting.

Presenting Research or Scholarship in a paper or a presentation at a Conference or Lecture (International)  
 Presenting Research or Scholarship in a paper or a presentation at a Conference or Lecture at a Conference or Lecture (Domestic)  
 Conducting Research or Scholarship (Individual Faculty Project)  
 Conducting Research or Scholarship (Enhancement of Academic Dept. / Program)  
 Attending Workshops, Seminars, and Conferences (Individual Faculty Development)  
 Attending Workshops, Seminars, and Conferences (Enhancement of Academic Dept. / Program)

8. Project Information:

Name of Conference, Organization, or Project:   
Title of Presentation or Project:   
Date of Presentation or Project:   
Location of Conference, Organization, or Project:

**9. Briefly State How Project Supports Tenure, Promotion, and /or the College's Strategic Plan:**

This research project involves the Photophysical studies of newly developed Porphyrinoid dyes appended with nitro groups for photodynamic therapy (PDT). The research project helps to establish a relation with four year college (Hunter College) and will also help our students to do research, present in a scientific conference and develop a habit of writing scientific reports.

**10. Abstract**

Provide a Description of Your Project, Including Subject Area, Purpose, and Major Activities:

Porphyrinoids decorated at their periphery with various number of nitro groups have been extensively investigated for wide range of applications such as in redox catalytic activity, nonlinear optical materials, theranostics, and in artificial solar energy harvesting devices. The substitution of a nitro group onto a porphyrin compound has a large effect on the photophysical properties and potential applications of these dye. We present here the spectroscopic studies of a series of nitrated porphyrinoids in polar (DMSO) and non polar (toluene) solvents. The nitro group on the porphyrins shown to decrease the fluorescence quantum yield as well as reduces the lifetime of the porphyrinoids. The amount of fluorescence quenching depends on the number and position of the nitro groups appended on the porphyrinoid macrocycle. The low fluorescence quantum yield is complementary of their high triplet quantum yield, makes these chromophores a potential platform to develop new photosensitizer for photodynamic therapeutic treatment of cancers. Nitro groups when present at the  $\beta$ -pyrrole position significantly affect the electronic properties and can interact with a nearby bulky meso substituent to significantly distort the porphyrin macrocycle compared to corresponding un-substituted porphyrin. We propose that molecular distortion due to steric hindrance is the prevailing cause behind all of the anomalous photophysics.

**11. Evaluation**

Discuss how you will determine if your project was successful (for example, future publication of a presentation, audience response, survey).

We have obtained very interesting results from this project that seems to be promising to develop next generation photosensitizer for PDT. The results attracted a wide variety of scientific community during my presentation at ACS meeting, Boston MA. We are in a process to write up a manuscript for result obtained and are planning to submit the work to a peer reviewed scientific journal in this academic year.

**9. Briefly State How Project Supports Tenure, Promotion, and /or the College's Strategic Plan:**

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**12. Budget**

Provide a complete budget that specifies the items for which the EDIT grant funds will be used. **Attach copies of receipts for all items requested.** In preparing your budget, review the Eligibility & Award Criteria section of this application (page 2) which lists the type of expenses funded by EDIT. Be sure to indicate whether you are providing the **ACTUAL** or **ESTIMATED** cost of an item. You may provide a limited number of estimated expenses for services not yet rendered for which your costs are estimated. For example, your travel takes place after the application deadline so you have estimated the cost of your taxi ride from the airport to the hotel. In this case, be sure to include the pending item(s) in your budget, submit your application by the deadline, and send the co-chairs copies of the missing items as soon as you get them. Full-time faculty requesting funds for conferences supported by Academic Affairs should request 60% of allowable expenses for **domestic conferences** and indicate you are doing so for each budget item. For **international conferences** request funds for items not covered by Academic Affairs. **Per diem requests will be granted only for conference presentations. EDIT only considers the expenses of the applicant.** If you are sharing expenses (hotel room, etc.), or traveling with others, please adjust your budget accordingly and make specific references to this in the notes section of the application (see Budget).

| Category     | Number of Items | Cost                | Actual or Estimated | 60% of Expenses? Yes / No |
|--------------|-----------------|---------------------|---------------------|---------------------------|
| Lodging      | 1               | \$531.50            | Actual              | yes                       |
| Auto Mileage | 1               | \$143.90            | Actual              | yes                       |
| Parking Fee  | 1               | \$75.60             | Actual              | Yes                       |
| Tolls        | 1               | \$10.33             | Actual              | Yes                       |
| Meals        | 1               | \$137.4             | Actual              | Yes                       |
|              |                 | \$                  |                     |                           |
|              |                 | \$                  |                     |                           |
| <b>Total</b> |                 | <b>\$898.729986</b> |                     |                           |

**Notes:**  
 1. The actual Lodging cost was \$885.87.  
 2. The total mileage was 440 miles ( 440 \* \$.554= \$ 239.80)  
 3. Total Parking Fee was \$126.00  
 4. Tolls were \$17.23  
 5. Total Meals expenses (as per diem for four stay at conference venue) = \$229.00

13. Amit Aggarwal   
 Applicant's Signature

9/25/2018  
 Date

\*\*\*\*FOR PART-TIME FACULTY ONLY\*\*\*\*

\_\_\_\_\_  
 Chairperson's signature  
 (Applicant has been in continuous service for the past two academic years – September through June)

\_\_\_\_\_  
 Date

6/13/2018

256th ACS National Meeting Scheduling Notice - Amit Aggarwal

## 256th ACS National Meeting Scheduling Notice

maps@services.acs.org

Wed 6/13/2018 11:37 AM

To: Amit Aggarwal [REDACTED]

Dear Amit Aggarwal,

Your presentation has been scheduled for the technical program of the 256th ACS National Meeting in Boston, MA, August 19-23, 2018.

PAPER ID: 2990479

PAPER TITLE: Effect of nitro group on the photophysical properties of porphyrin dyes (final paper number: INOR 735)

DIVISION: Division of Inorganic Chemistry

SESSION: Chemistry of Materials

SESSION TIME: 5:30 PM - 7:30 PM

PRESENTATION FORMAT: Poster

DAY & TIME OF PRESENTATION: Wednesday, August 22, 2018, 5:30 PM - 7:30 PM

ROOM & LOCATION: Exhibit Hall B2/C - Boston Convention & Exhibition Center

### Registration Required

In order to make your presentation, you must be registered for the Boston, MA meeting. Early registration is open and discounts are available through midnight EDT July 9, 2018. Registration rates and policies are available at [www.acs.org/bostoninfo](http://www.acs.org/bostoninfo).

### Housing Available

ACS has secured discounted hotel room rates in each of the conference hotels. Free internet and complimentary shuttle buses are available. Please visit [www.acs.org/bostoninfo](http://www.acs.org/bostoninfo) to view the technical session locations and book your housing beginning May 21, 2018.

### Cancellation or Withdrawal

If you are unable to give your presentation, please send an email with your name, paper ID, paper title, and the division you were presenting in to [maps@acs.org](mailto:maps@acs.org). If you have questions about your presentation, please contact your program chair (see <https://callforpapers.acs.org/boston2018> for contact information).

If you have already registered or booked your hotel room, please visit [www.acs.org/bostoninfo](http://www.acs.org/bostoninfo) to read the cancellation policy for registration and housing.

### International Attendees and Visa Procurement

If you require a visa to travel to the U.S., the U.S. Department of State recommends starting the process at least three months before the departure date. Further information on the visa process can be found by visiting the U.S. Department of State or the ACS National Meeting & Exposition international registrant page. [REDACTED]

Please note that ACS is neither responsible nor liable if a visa is denied or delayed. If your visa decision is still pending on or after July 9, 2018, please consider sending an email to [intlacts@acs.org](mailto:intlacts@acs.org) explaining your status and visiting the U.S. National Academies International Visitor Office to complete their visa questionnaire at [http://sites.nationalacademies.org/PGA/biso/visas/PGA\\_048197](http://sites.nationalacademies.org/PGA/biso/visas/PGA_048197).

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**PROGRAM BOOK**



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682. Catalytic upgrading of ethanol using pincer type complexes. *R.M. Padilla, E. Christensen, M. Nielsen*

683. Catalytic synthesis of "super" linear alkenyl arenes using a Rh(I) catalyst supported by a "capping arene" ligand: Access to aerobic catalysis. *J. Chen, R.J. Nielsen, W.A. Goddard, B.A. McKeown, T. Gunnoe*

684. Theoretical study on the reaction mechanisms of platinum-catalyzed acylation reaction. *E. Warden, L.J. Bartolotti, Y. Li, S. Huo*

685. Palladium-catalyzed allylic alkylation of 2-aryl-1,3-dithianes, an umpolung synthesis of  $\beta,\gamma$ -unsaturated ketones. *N. Trongirawat*

686. Synthesis of high oxidation state Mo=CHX complexes (X = Cl, CF<sub>3</sub>, CN) relevant to Z-selective electron poor olefin metathesis. *S. Venkatramani, K. Bukhryakov, R.R. Schrock, A.H. Hoveyda, C. Tsay, P. Mueller*

687. Synthesis of molybdenum oxo alkylidene complexes through addition of water to alkylidyne complexes. *F. Zhai, K. Bukhryakov, R.R. Schrock*

688. Zirconium MOF hydrates: Remediating organophosphorus contaminants. *Y. Kalinovsky, B. Blight, S.J. Holder, N.J. Cooper, M. Main*

689. Study of axial steric effects on reductive elimination from (PNP)Rh<sup>III</sup> complexes. *S. Gu, K.H. Taylor, J. Chen, G. Fortman, R.J. Nielsen, W.A. Goddard, T. Gunnoe*

690. Exploring C-N coupling promoted at group 4 metal centers. *D. Javier Jimenez, A. Kreider-Mueller, D.R. Manke*

691. Comparative nitrene-transfer chemistry to olefinic substrates mediated by a library of anionic Mn(II) triphenylamido-o-amine reagents and M(II) congeners (M = Fe, Co, Ni): An experimental and computational study. *Z. Sun, A. Khatra, T.R. Cundari, P. Stavropoulos*

692. Chemical and electrochemical activation modes of a [Cp\*<sub>2</sub>Rh] monohydride. *E. Boyd, K.V. Prather, D. Lionetti, J.D. Blakemore*

693. Multifunctional aryloxide  $\beta$ -diketiminato rare-earth complexes for the ring-opening polymerization of cyclic esters. *K.C. Casey, J.K. Appiah, J.R. Robinson*

**SECTION B**  
*Boston Convention & Exhibition Center  
 Exhibit Hall B2/C*

**Organometallic Chemistry: Applications to Organic Transformations**  
*N. S. Radu, Organizer  
 5:30 – 7:30*

694. C-C and C-heteroatom coupling reactions at high valent nickel. *C. Roberts, N. Camusso, E. Bowes, M.S. Sanford*

695. Non-directed C-H activation and formation of C-N and C-O bonds using Cp\*Ir and Cp\*Rh catalysts. *M. Kerr, E. Hickey, E. Mattson, S. Rosario, V. Fratantonio*

696. Development of palladium-catalyzed allylation of aromatic imidates. *S.R. Wootzig, B. McLarnon, P. O'Connor*

**SECTION C**  
*Boston Convention & Exhibition Center  
 Exhibit Hall B2/C*

**Coordination Chemistry: Characterization & Applications**  
*A. Larsen, Organizer  
 5:30 – 7:30*

697. Density functional theory study of potential NO donors [RuCl(NO)(cyclam)]<sup>+</sup> and [Ru(EDTA)NO]. *J. Joralan, C. Cebigan*

698. Effects of intramolecular spin polarization on the thermodynamic properties of tetraoxalene exchange-coupled systems. *S. Li, J.K. McCusker*

699. A new set of Cu(II) coordination polymers with mixed ligand of dicarboxylate and pyridyl substituted diaminotriazine: selective sorption towards CO<sub>2</sub> and cationic dye. *S. Chand*

700. Rhodamines-functionalized silsesquioxanes cages as optical sensor for highly sensitive and selective detection of Hg<sup>2+</sup> ion in aqueous solution. *P. Piyanch, R. Kuntham, V. Ervithayosuporn, N. Wanichacheva*

701. A highly selective ON-OFF fluorescence detection of Cu<sup>2+</sup> ions in aqueous solution based on core-substituted naphthalene diimides (cNDIs). *P. Praikaeuw, S. Langford, S. Maniam, J. Sinrak, N. Wanichacheva*

702. Aluminum and titanium metal complexes: Synthesis, characterization and their application in ring opening metathesis polymerisation (ROMP). *R. Lord, F. Janeway, P. McGowan*

703. Coupling UV-Vis and NMR titration models to determine association constants of arylazothioformamide ligands with various copper(I) salts. *S.R. Wolfe, M. Chakraborty, N.A. Johnson, N.J. Rube, C. Kingsley, M.F. Roll, K.V. Waynant, J. Moberly*

704. Molybdenum nitride basicity effects on nitrogen reduction. *A. Hickey, C. Tsay, P. Mueller, R.R. Schrock*

705. Supramolecular complexes of nucleotides with a macrocycle-based molecular host. *A. Hossain, M. Rhaman, A. Jahan, D.R. Powell*

706. Selective binding of cyanide with a dinuclear metal complex. *A. Alamgir, M. Rhaman, D.R. Powell, A. Hossain*

707. Cu(II) and Zn(II) complexes of 4-hydroxy-N-[(3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl)methylene] benzohydrazide: Synthesis, characterization, DNA binding, DNA cleavage and antibacterial studies. *V. Chitreddy*

708. Coordination number effects on copper-mediated aliphatic carbon-carbon bond cleavage reactions of chlorinated  $\beta$ -diketonates. *J.G. Elsberg, S. Saraf, L.M. Berreau*

709. Transition metal ion encapsulation via micelles of diblock copolymers. *C. Chen, A. Ringuette, H. Koata, L. Cai, S.L. Goh, C. Goh*

710. Properties, reactivity, and applications of trans-dichlorobis(ethylenediamine)cobalt(III) chloride, trans-[Co(en)<sub>2</sub>Cl<sub>2</sub>]. *C.S. Lin Latt, J.P. Lanorio*

711. Organophosphate sensing using the 3d metal coordination complexes. *S. Love, I. Bhattachick*

712. Transition metal complexes: Toward catalysis and small molecule therapy. *E. Delgado, E.R. Pouison, D.B. Grotjahn*

713. Development of macrocyclic Fe(III) T. MRI contrast agents. *D. Asik, E. Snyder, J. Spornyak, J.R. Morrow*

714. Copper based organometallic light-emitting luminophores. *Y. Kim, Y. Lee*

**SECTION D**  
*Boston Convention & Exhibition Center  
 Exhibit Hall B2/C*

**Chemistry of Materials**  
*C. G. Lugmair, Organizer  
 5:30 – 7:30*

715. Stable homo-interpenetrated triazolate-based MOF for H<sub>2</sub> storage. *Q. Wang, H. Zhou*

716. Fabrication of  $\alpha$ -Fe<sub>2</sub>N catalytic sites in porous carbons derived from an iron-triazolate crystal. *Y. Fujiwara, M. Tsujimoto, K. Konokwan, N. Tabari, S. Horike, S. Kitagawa*

717. Highly sensitive, transparent, and flexible temperature sensors based on silver fractal dendrites. *J. Kim, Y. Lee*

718. Silver nanoparticle inks for fine patterns using reverse offset printing. *K. Park, Y. Lee*

719. Design and applications of dendritic ligands for nanoparticle stability, assembly, and property tuning. *K.C. Elbert, J.D. Lee, N.M. Kroak, D. Jishkariani, Y. Wu, C.B. Murray*

720. Porous gold nanoparticles for inhibiting viral membrane fusion of Influenza A virus. *J. Kim, S. Haom, D. Song*

721. Design of extended phosphonate ligands to increase porosity and stability of metal-organic frameworks. *W.S. Pantaja Romero, V. López-Mejias*

722. Efficient thermal atomic layer deposition process enhancing by precursors containing long chains electron-donating ligand. *Y. Zhang, L. Du, Y. Ding*

723. Modified silicon nanoparticles as advanced anode materials and the improved electrochemical performance for lithium-ion battery. *N. Bao, Y. Liu, C. Zhong, J. Tian*

724. Synthesis and characterization of ZnO nanoparticles and their use to photocatalyze the degradation of malachite green. *A.E. Harris, C.C. Pena, J.E. Cowan, J.D. Harris*

725. Electrochemiluminescence of Ru doped metal-organic frameworks. *Q. Luoguo, M. Cai, A.J. Morris*

726. Thermal decomposition of [Cat]<sup>+</sup>[WSe<sub>6</sub>]<sup>-</sup> for facile formation of WSe<sub>2</sub>. *J. Kim, B. Park, T. Chung, C. Kim*

727. Electrochemical reductive grafting and photothermal properties studies of bis(diazonium) gold(III) salts. *S. Isah, B. Warkie, A. Marciano, S. Panicker, A. Mohamed*

728. Mesoporous NNN-pincer metal-organic framework as readily prepared noble metal-free catalyst. *Y. Zhang, J. Li, X. Yang, H. Zhou*

729. 2-Hydroxy-4-methoxybenzophenone-5-sulfonate intercalated layered double hydroxide: 2D restriction-induced luminescence and its application as a fluorescent biosensor. *J. Lu, R. Ma, P. Zhang*

730. Synthesis and design of new type 3 porous liquids. *J. Cahir, M. Tsang, S. James, J. Jacquemin, D. Rooney*

731. Zeolite-supported bismuth oxyiodide visible-light-active photocatalysts for dehydrochlorination of cyclohexane. *R. Arthur, R. Warner, C. Vaughn, J. Hamilton, H.H. Patterson*

732. Solvothermal synthesis of FeSe-SrTiO<sub>3</sub> nanocomposites and their magnetic properties. *K. Kim, S. Huh, K. Song, H. Park, Y. Sur, K. Kim, N.H. Hur*

733. Solvent-free synthesis of nitrogen-doped carbon sheets derived from glucose for CO<sub>2</sub> capture. *K. Lee, S. Lee, H. Kim, S. Bang, B. Lee, N.H. Hur*

734. Fabricating iron oxide magnetic features using an iron MOD coordination complex by inkjet printing. *O. Almalki, S. Williams*

735. Effect of nitro group on the photophysical properties of porphyrin dyes. *A. Aggarwal*

736. Atmospheric-pressure sulfur-based microplasma for material synthesis. *F. Zoghieb, S. Stephen, S. Al Hassan*

737. Solution phase synthesis of highly crystalline Bi chalcogenide nanostructured materials. *V.V. Pillai, V. Tzitzios, S. Stephen, S. Al Hassan*

738. Red phosphorus thin films for energy applications. *P. Martins Amaral, H. Ji, G. Schwenk*

739. Using metal-organic frameworks as multi functional platforms for the studies of medicinal and cosmetic materials. *M. Zhuo, Y. Chen*

740. Solvothermal synthesis of pure-phase NU-901: The effects of zirconium salt and carboxylic modulator components on MOF topology and phase purity. *S.J. Garibay, T. Islamoglu, O.K. Farha, J. DeCoste*

741. Synthesis and characterization of lead halide perovskites for solid state lighting. *E.T. Nguyen, D.A. Hardy, R.A. Tigao, G.F. Strouse*

742. Conductivity of borane salts: Characteristics of amino borane cages and hydroxylated versions. *D. Staska, G. Bosworth, C. Hillebrand, J.N. Woodford*

743. Incorporation of corrole and porphyrin based ligands into metal-organic frameworks. *J. Alatis*

744. Comparative toxicity of ZnO nanoparticles synthesized using different amines. *J.D. Harris, C.C. Pena, J.E. Cowan, K. Cornell*

745. Study of haziness in silica wet-gels and in mechanically strong, thermally insulating polymer-crosslinked aerogels. *C. Mandal, S. Donthula, C. Satriou-Leventis, N. Leventis*

746. Structural reorganization of silica wet-gels upon drying: Why aerogels shrink? *C. Mandal, S. Donthula, C. Satriou-Leventis, N. Leventis*

747. Design and synthesis of WO(OR)<sub>2</sub>L precursors for chemical vapor deposition of WO<sub>3</sub> films. *X. Su, D.C. Back, L. McElwee-White*

748. Sturdy, monolithic SiC and Si<sub>3</sub>N<sub>4</sub> aerogels from compressed polymer-crosslinked silica xerogel powders. *P. Rewatkar, T. Taghvaei, A. Saeed, S. Donthula, C. Mandal, N.K. Chandrasekaran, T. Leventis, S. T. K. C. Satriou-Leventis, N. Leventis*

749. Fabrication and characterization of cerium-copper-silica and cerium-copper-alumina catalytic aerogels. *T.F. Andre, M.K. Carroll, A.M. Anderson, B.A. Bruno*

750. Electrode-assisted synthesis (EAS) of metal-organic frameworks. *A. Antonia, E.D. Bloch, J. Rosenthal*

751. Functionalization of UiO-66 MOF composites to enhance catalytic performance for the photoelectrochemical water splitting cell. *J.J. Shanahan, D.S. Kissel, J.J. Kelleher*

752. Exploring the electrocatalysis of MIL-100(Fe) derivatives. *A.J. Arnoff, E.D. Bloch, J. Rosenthal*

753. Heterodinuclear metal-organic framework materials for photocatalytic carbon dioxide reduction. *H. Brooks, B. Yan*

**SECTION E**  
*Boston Convention & Exhibition Center  
 Exhibit Hall B2/C*

**Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals**  
*N. S. Radu, Organizer  
 5:30 – 7:30*

754. Reimagining early transition metal luminescent metallocenes with built-in reactive ligands. *P.N. Do, M.E. Nally, Y. Zhang, C. Millsman*

755. Constructing a scandocene donor series with <sup>45</sup>Sc solid state NMR. *D. Culver, W. Huynh, M.P. Conley*

# Registration Information - ACS Fall National Meeting 2018

ACS Fall National Meeting 2018 <eventconfirmation@xpressreg.net>

Wed 8/22/2018 5:32 PM

To: Amit Aggarwal <Aaggarwal@lagcc.cuny.edu>

## 256th American Chemical Society National Meeting and Exposition - Onsite Registration Receipt

---

### Contact Information

Badge Number: 215520

Reg Type:

Name: AMIT AGGARWAL

Company: CUNY LAGUARDIA

Address: [REDACTED]

City: [REDACTED]

State/Province: NY

Zip/Postal Code: [REDACTED]

Country: United States

Phone: [REDACTED]

Email: [REDACTED]

### Registration Detail

| Badge  | Name          | Registration Class  |
|--------|---------------|---|
| 215520 | AMIT AGGARWAL | NonMember Wednesday<br>1 - (WDN) Wednesday NonMember - \$570.00 |

### Financial Summary

Item Total: \$570.00

Amount Paid: \$0.00

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Balance Due: \$570.00



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Amit Aggarwal  
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Page Number : 1 Invoice Nbr : -1  
 Guest Number : 5206588  
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 Arrive Date : 20-AUG-18 18:31  
 Depart Date : 23-AUG-18 12:00  
 No. Of Guest : 1  
 Room Number : 1452  
 Club Account :

Tax Invoice

Tax ID : 26-1482881

Sheraton Boston AUG-23-2018 09:55 CWONG191

| Date        | Reference | Description               | Charges (USD) | Credits (USD) |
|-------------|-----------|---------------------------|---------------|---------------|
| 20-AUG-18   | RT1452    | Room Chrg Grp Association | 258.00        |               |
| 20-AUG-18   | RT1452    | State Tax                 | 14.71         |               |
| 20-AUG-18   | RT1452    | Occupancy/Tourism Tax     | 7.10          |               |
| 20-AUG-18   | RT1452    | City Tax                  | 15.48         |               |
| 21-AUG-18   | RT1452    | Room Chrg Grp Association | 258.00        |               |
| 21-AUG-18   | RT1452    | State Tax                 | 14.71         |               |
| 21-AUG-18   | RT1452    | Occupancy/Tourism Tax     | 7.10          |               |
| 21-AUG-18   | RT1452    | City Tax                  | 15.48         |               |
| 22-AUG-18   | RT1452    | Room Chrg Grp Association | 258.00        |               |
| 22-AUG-18   | RT1452    | State Tax                 | 14.71         |               |
| 22-AUG-18   | RT1452    | Occupancy/Tourism Tax     | 7.10          |               |
| 22-AUG-18   | RT1452    | City Tax                  | 15.48         |               |
| 23-AUG-18   | MC        | Mastercard-1329           |               | -885.87       |
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Amit Aggarwal  
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| Guest Number | : | 5206588   |             |   |    |
| Folio ID     | : | A         |             |   |    |
| Arrive Date  | : | 20-AUG-18 | 18:31       |   |    |
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# Effect of Nitro Group on the Photophysical Properties of Porphyrin Dyes

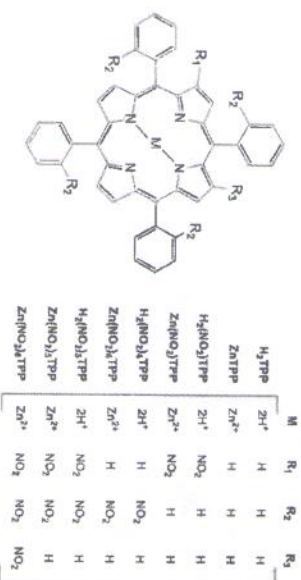
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## Abstract

Porphyrinoids decorated at their periphery with various number of nitro groups have been extensively investigated for wide range of applications such as in redox catalytic activity, nonlinear optical materials, theranostics, and in artificial solar energy harvesting devices. The substitution of a nitro group onto a porphyrin compound has a large effect on the photophysical properties and potential applications of these dye. We present here the spectroscopic studies of a series of nitrated porphyrinoids in polar (DMSO) and non polar (toluene) solvents. The nitro group on the porphyrins shown to decrease the fluorescence quantum yield as well as reduces the lifetime of the porphyrinoids. The amount of fluorescence quenching depends on the number and position of the nitro groups appended on the porphyrinoid macrocycle. The low fluorescence quantum yield is complementary of their high triplet quantum yield, makes these chromophores a potential platform to develop new photosensitizer for photodynamic therapeutic treatment of cancers. Nitro groups when present at the  $\beta$ -pyrrole position significantly affect the electronic properties and can interact with a nearby bulky meso substituent to significantly distort the porphyrin macrocycle compared to corresponding un-substituted porphyrin. We propose that molecular distortion due to steric hindrance is the prevailing cause behind all of the anomalous photophysics.

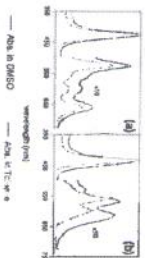
## Structure of Nitro Porphyrinoids studied



## Expectations for Nitro-Porphyrin Dyes

- Nitro groups are strongly electron withdrawing. They polarize the porphyrin macrocycle, causing changes in the photophysics including red shifts, quenching etc.
- Nitro groups can lead to intramolecular charge transfer (ICT) states.
- The kinetics of ICT states and the spectroscopic properties can both be controlled by changing the position and number of nitro groups on the macrocycle.
- NO<sub>2</sub> can promote both internal conversion to the ground state, and intersystem crossing to triplet states.

## Absorption Spectra



Normalized UV-Vis absorption spectra of the free base (a, H<sub>2</sub>(NO<sub>2</sub>)TPP) and metalated (b, Zn(NO<sub>2</sub>)TPP) nitroporphyrin in DMSO (black lines) and toluene (red lines).

## Emission Spectra



Normalized fluorescence emission spectra of the free base (a, H<sub>2</sub>(NO<sub>2</sub>)TPP) and metalated (b, Zn(NO<sub>2</sub>)TPP) nitroporphyrin in DMSO (black lines) and toluene (red lines). Degraded N<sub>2</sub> solvents are denoted by solid lines, and those under ambient atmosphere are denoted by dashed lines, although they overlap due to normalization.

## Fluorescence Quantum yield

TPP and ZnTPP were used as a reference,  $\Phi_F = 0.11$  and 0.030 for TPP and Zn-TPP in Toluene, respectively.

$$\Phi_S = \Phi_R \times \frac{I_{int} S_R}{I_{int} S_S}$$

where  $\Phi$  is fluorescence quantum yield, A is absorbance, and I is fluorescence area under curve. S and R represents sample and reference respectively.

## 3D model Structure of nitro Porphyrin



Table: Steady state fluorescence emission and lifetime data for the por compounds in toluene and DMSO.

| Compound   | Emission (nm) | Quantum Yield (%)  |                    | Lifetime under Air |                   | Lifetime under N <sub>2</sub> |                   |
|--|---------------|--------------------|--------------------|--------------------|-------------------|-------------------------------|-------------------|
|  |               | Air                | N <sub>2</sub>     | $\tau_1$ , ns (%)  | $\tau_2$ , ns (%) | $\tau_1$ , ns (%)             | $\tau_2$ , ns (%) |
| <b>Free Base Porphyrins in Toluene</b>             |               |                    |                    |                    |                   |                               |                   |
| H <sub>2</sub> TPP                                 | 613, 719      | 0.112              | 0.110              | 9.53               | 912               | 12.5                          | 922               |
| H <sub>2</sub> (NO <sub>2</sub> ) <sub>1</sub> TPP | 580           | 0.060              | 0.060              | 1.36 (1.9%)        | 114 (0.4%)        | 1.85 (2.1%)                   | 125 (1.8%)        |
| H <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub> TPP | 621, 518      | 0.045              | 0.048              | 1.87 (3.2%)        | 12 (0.3%)         | 2.28 (2.9%)                   | 122 (1.1%)        |
| <b>Free Base Porphyrins in DMSO</b>                |               |                    |                    |                    |                   |                               |                   |
| H <sub>2</sub> TPP                                 | 592, 715      | 0.112              | 0.112              | 922                | 1112              | 922                           | 1112              |
| H <sub>2</sub> (NO <sub>2</sub> ) <sub>1</sub> TPP | 608, 696, 714 | 0.230              | 0.230              | 0.42 (1.4%)        | 11.9 (0.9%)       | 0.47 (2.1%)                   | 11.5 (0.8%)       |
| H <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub> TPP | 685           | 0.143              | 0.143              | 2.20 (3.8%)        | 3.40 (2.1%)       | 0.77 (0.9%)                   | 3.35 (2.1%)       |
| <b>Zinc Porphyrins in Toluene</b>                  |               |                    |                    |                    |                   |                               |                   |
| ZnTPP  | 596, 645      | 0.030 <sup>a</sup> | 0.030 <sup>a</sup> | 2.59 <sup>a</sup>  | 922               | 922                           | 922               |
| Zn(NO <sub>2</sub> ) <sub>1</sub> TPP              | 591           | 0.030              | 0.031              | 1.37 (0.7%)        | 6.63 (0.4%)       | 1.30 (1.3%)                   | 6.55 (2.1%)       |
| Zn(NO <sub>2</sub> ) <sub>2</sub> TPP              | 567           | 0.030              | 0.030              | 1.20 (1.2%)        | 4.12 (0.1%)       | 1.18 (0.9%)                   | 5.83 (1.1%)       |
| Zn(NO <sub>2</sub> ) <sub>3</sub> TPP              | 553, 715      | 0.031              | 0.031              | 0.45 (2.1%)        | 1.57 (0.8%)       | 1.37 (0.4%)                   | 1.93 (0.6%)       |
| <b>Zinc Porphyrins in DMSO</b>                     |               |                    |                    |                    |                   |                               |                   |
| ZnTPP  | 607, 610      | 0.039 <sup>a</sup> | 0.039 <sup>a</sup> | 922                | 1.92 <sup>a</sup> | 922                           | 922               |
| Zn(NO <sub>2</sub> ) <sub>1</sub> TPP              | 602, 595      | 0.212              | 0.212              | 0.92 (3.8%)        | 4.40 (0.3%)       | 0.93 (0.8%)                   | 5.77 (1.2%)       |
| Zn(NO <sub>2</sub> ) <sub>2</sub> TPP              | 553           | 0.203              | 0.203              | 0.23 (0.2%)        | 11.15 (1.1%)      | 0.21 (0.2%)                   | 1.54 (1.8%)       |
| Zn(NO <sub>2</sub> ) <sub>3</sub> TPP              | 518, 713      | 0.032              | 0.030              | 1.17 (2.9%)        | 4.87 (0.4%)       | 1.20 (1.9%)                   | 3.31 (0.9%)       |

Note: The steady-state excitation wavelength was  $\lambda_{exc} = 414$  nm for toluene and  $\lambda_{exc} = 412$  nm for DMSO. For lifetimes, excitation was at  $\lambda_{exc} = 405$  nm and emission was detected at  $\lambda_{em} = 651$  nm.

Table: DFT calculated ground state physical data for free base  $\beta$ -nitro-Por compounds

| Conformer <sup>a</sup>                              | Phenyl Group Angles <sup>b</sup> |             |             | Nitro Angle <sup>c</sup> | Energy <sup>d</sup> (kcal/mol) | Dipole Moment <sup>e</sup> (D) |
|---|----------------------------------|-------------|-------------|--------------------------|--------------------------------|--------------------------------|
|   | $\tau_{12}$                      | $\tau_{13}$ | $\tau_{23}$ |                          |                                |                                |
| <b>H<sub>2</sub>(NO<sub>2</sub>)TPP</b>             |                                  |             |             |                          |                                |                                |
| Rot1e   | 90°                              | 90°         | 90°         | 90°                      | 920                            | 910                            |
| Rot. 1  | 61°                              | 70°         | 66°         | 76°                      | 1,297                          | 7.45                           |
| Rot. 2  | 60°                              | 75°         | 69°         | 55°                      | 41°                            | 7.82                           |
| Rot. 3  | 58°                              | 64°         | 70°         | 75°                      | 0.929                          | 7.75                           |
| Stable  | 57°                              | 61°         | 63°         | 61°                      | 0.000                          | 7.83                           |
| <b>H<sub>2</sub>(NO<sub>2</sub>)<sub>1</sub>TPP</b> |                                  |             |             |                          |                                |                                |
| Rot1e   | 68°                              | 84°         | 80°         | 77°                      | 39°                            | 10.58                          |
| Rot. 1  | 67°                              | 84°         | 79°         | 76°                      | 38°                            | 1.419                          |
| Rot. 2  | 68°                              | 84°         | 80°         | 77°                      | 39°                            | 9.40                           |
| Rot. 3  | 67°                              | 79°         | 83°         | 78°                      | 38°                            | 1.163                          |
| Rot. 4  | 68°                              | 80°         | 80°         | 77°                      | 40°                            | 1.466                          |
| Rot. 5  | 70°                              | 80°         | 80°         | 78°                      | 37°                            | 0.337                          |
| Rot. 6  | 70°                              | 81°         | 80°         | 78°                      | 37°                            | 22.90                          |
| Rot. 7  | 71°                              | 81°         | 80°         | 77°                      | 39°                            | 0.223                          |
| Rot. 8  | 71°                              | 83°         | 80°         | 80°                      | 38°                            | 0.325                          |
| Rot. 9  | 71°                              | 84°         | 80°         | 80°                      | 38°                            | 0.183                          |
| Rot. 10   | 71°                              | 84°         | 81°         | 77°                      | 37°                            | 0.000                          |

## Conclusions

- The presence of nitro group significantly quenches the fluorescence as well as reduces the lifetime of the porphyrinoid.
- The strong electron withdrawing nature of the nitro group makes it very useful for modulating the ground state properties and excited state dynamics of porphyrinoids and other organic dyes.
- A nitro group at a  $\beta$ -pyrrole position can interact with a nearby bulky meso-substituent to significantly distort the macrocycle.
- The position of the nitro group will significantly modify the excited state dynamics.

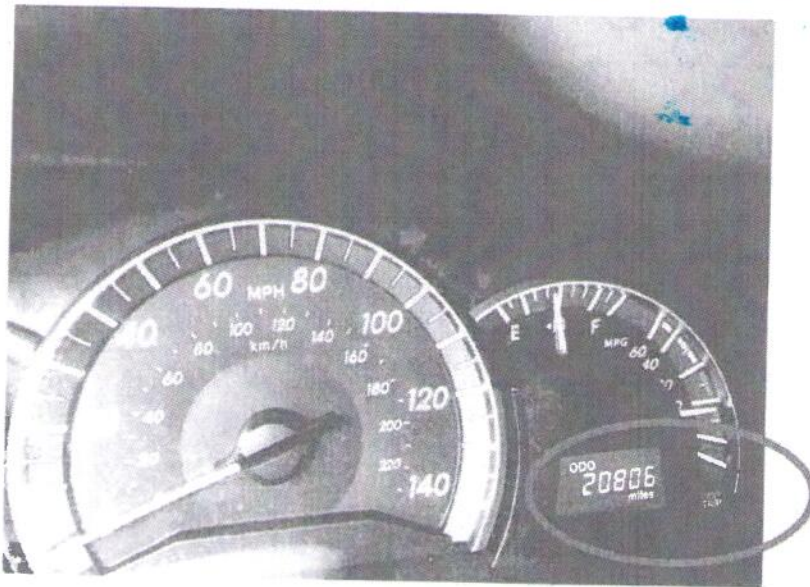
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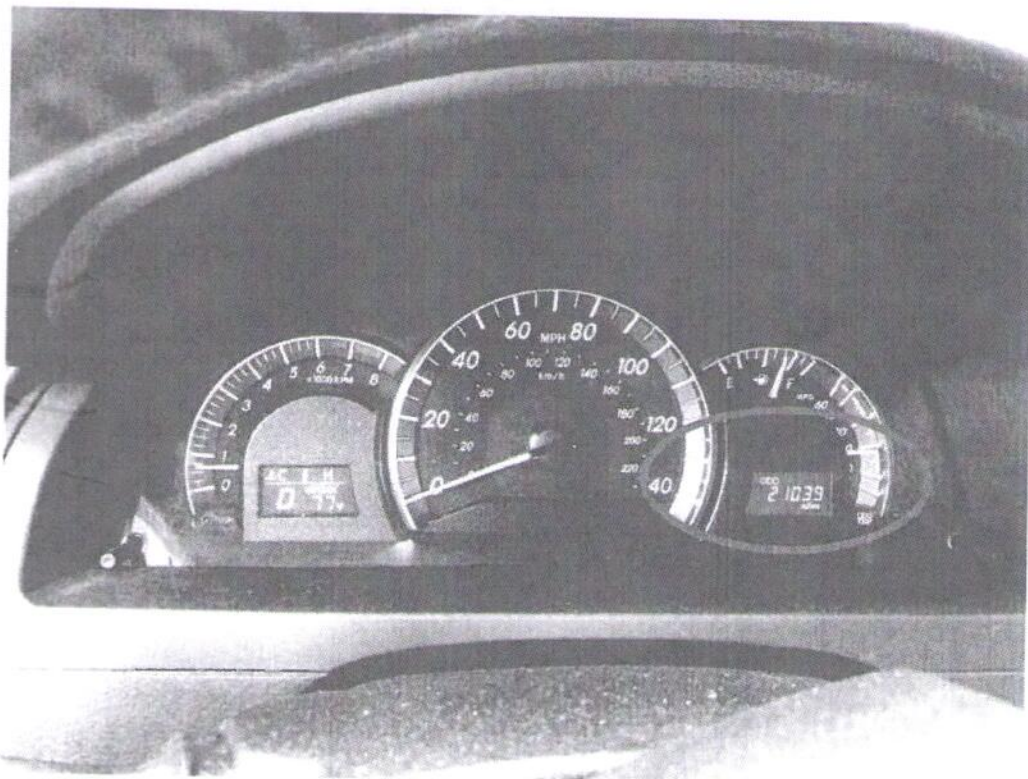
## Acknowledgement

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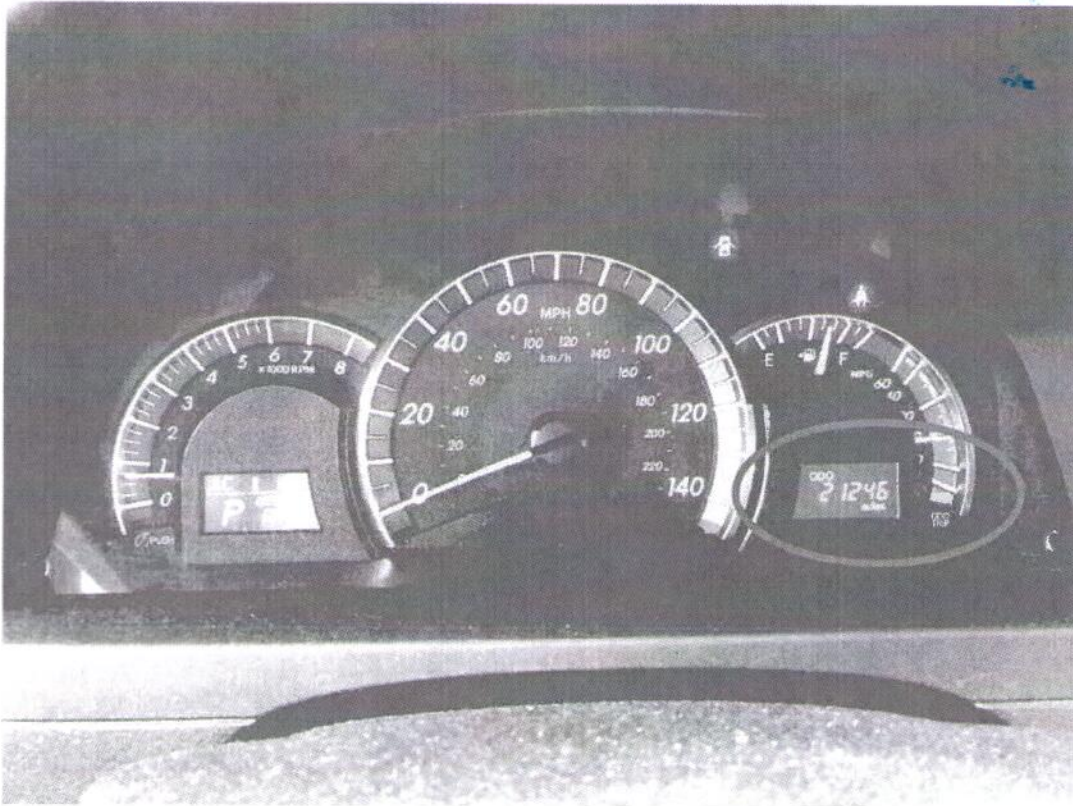
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Car Odometer Reading at the Final destination Point (Shareton Boston Hotel, Boston, MA)



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| 08/23/2018   | 08/20/2018       | 00811778949      | MassDOT | TOLL                | 16:43:22   | 126         | 03         | 16:50:07  | 131        | 03        | 2                 | \$2.65    | Y        | STANDARD  | N         | \$18.12 |
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| 08/20/2018   | 08/20/2018       | -                | MTAB&T  | Prepaid Adj Cr      | -          | -           | -          | 14:58:35  | -          | -         | -                 | \$10.00   | Y        | -         | -         | \$28.19 |
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| 08/22/2018   | 08/20/2018       | 00811778949      | NVSTA   | TOLL                | -          | -           | -          | 11:52:58  | NIR        | 08N       | 2L                | \$1.66    | Y        | STANDARD  | N         | \$20.77 |
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**APPENDIX E: PERSONAL VEHICLE TRAVEL RECORD**

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|---------------|--|--|----------------|-----------------|------------------------|
| 8/20          | 20806  | 21039                                    | 233            | 0.545           | \$ 126.99              |
| 8/23          | 21039  | 21246                                    | 207            | 0.545           | \$ 112.82              |
|               |  |  |                |                 | \$ 0.00                |
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|               |  |  |                |                 | \$ 0.00                |
|               |  |  |                |                 | \$ 0.00                |
| <b>TOTALS</b> |  |  |                |                 | \$ 239.80              |

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**Employee Signature** \_\_\_\_\_ **Date** \_\_\_\_\_