

Indian Science Technology and Engineering facilities Map (I-STEM)

Invites application for

1. Partial financial support for using R&D facilities in other institutions through the I-STEM web portal to Users from Academic Institutions and Start-ups (Format-1)

Format for requesting support for accessing and using facilities through the I-STEM web portal.

(i) Details of the Personal Information

- a. Name of the Faculty Member -**Dr. Alope Kumar Ghosh**
- b. Name of the Institution/Start-up-**Prabhat Kumar College, Contai**
Post- Karkuli, P.S.- Contai
Dist- Purba Medinipur, PIN - 721 404,
West Bengal, India
- c. Name of the Department-**Department of Chemistry**
- d. Degree registered for/Product being developed (for start-up) –**NA**

(ii) Mob. No.-**9902442354**, Email ID: **akghosh1982@gmail.com**

(iii) Project/Research topic Details:

a. Project Title/Research Title: **“Design, Synthesis and Structural characterization of nano-level sized novel 3d/4d transition metal clusters: Magnetic, DNA binding and Nuclease activity study”**

b. Sub area: Inorganic Chemistry

c. Area Description: Material science, Inorganic Chemistry which are dealt with strong magnetic materials that can be up taken by high tech data storage companies.

d. Aims & Objective (in Bullets): We have planned to investigate the use of different polynucleating ligands to produce some mono, di-, tri- and even polynuclear species. We emphasized on the formation of multinuclear systems with 3d/4d transition metals like Ti, Mn, Fe, Co, Ni, Cu/Zr, Nb, Mo and Y etc. We have also plan to study their single molecule magnetic (SMMs) properties, biological activity (anticancer, antimicrobial, antioxidant) and nature of metal ions and supporting co-ligands in presence of different N, O donor ligands

e. Duration (MM/YYYY): 04.2022-12.2025

f. Project Summary (1000 words):

Our first aim is to synthesize the salen or ethylenediimine/tetraethylenepentaimmine including 2,6-diethyl-4-methylphenol /salicylaldehyde moiety type of ligands¹. Secondly we have planned to synthesize novel 3d/4d (Ti, Mn, Fe, Co, Ni, Cu/Zr, Nb, Mo, Y) transition metal clusters either homo or hetero nuclear with the help of above synthesized ligands. Thirdly, we have also aimed to synthesize new core of metal cluster (complex) using commercial available ligands like 1,3,5-tris (4-carboxy phenyl)benzene, 3,5-dinitro benzoic acid, N-(2-hydroxyethyl) iminodiacetic acid and 3,3-dicarboxylic acid-2,2-biquinoline. Fourthly, the periphery of metal cluster should be of different organic/inorganic hybrid materials or metal organic framework (MOF)₂ compounds in nano-scale molecular sizes. Fifthly, Study the application of biological activity (anticancer, antimicrobial, antioxidant)³ by synthesized clusters. And lastly we will also study the single molecule magnetic (SMMs)⁴ properties of the synthesised clusters. After all we published high quality impact journal. Few experiments are illustrated here

$M(NO_3)_2$ ($M = Ni, Cu, Co$), $Mn(CH_3COO)_2 \cdot 4H_2O$ and solid I_2 (2:1:2) in $CH_3COOH/Pyridine$ (10/20,v/v) is added and stirred for 1h. The resulting solution is filtered and the filtrate is kept in slow evaporation for crystallization and complex is isolated. Stirred solution of 3,5-dnba, 2-pyridinemethanol and $M(NO_3)_2 \cdot 6H_2O$ ($M = Ni, Cu, Co$) (2:2:1) is added in $MeOH/MeCN$ (10:10; v/v) and reflux for about 3 hrs. The resulting solution was cooled at room temperature and filtered. The complex was crystallized and isolated. $Mn(ClO_4)_2 \cdot 6H_2O$, $[ZrO(NO_3)_2 \cdot 9H_2O$ or $Ti(isopropoxide)]$, 2,6-pyridine dimethanol and NaN_3 (3:1:1:1) in $MeOH/C_6H_5Me$ (18/2, v/v) is added with constant stirring for 30min. During stirring time solid $NnBu_4MnO_4$ is added in small portions and filtered, the filtrate is left undisturbed condition at room temperature and complex is isolated. Reaction of $Y(NO_3)_3 \cdot 6H_2O$, $Mn(NO_3)_2$ and solid I_2 in (1:1:1) molar ratio in $CH_3COOH/Pyridine$ (10/20,v/v) with stirred for half an hour and a make clear solution and kept it with undisturbed condition. After that crystal was appeared. Reaction of separately or mixture of $M(NO_3)_2$ ($M = Mn, Fe, Co, Ni, Cu$) and $M'(NO_3)_3$ ($M' = Zr, Nb, Mo, Y$) with synthesized salen Ligand I/II (1:1:2) in $MeCN/MeOH$ (10/20,v/v) in different condition with stirred for half an hour and a make clear solution and kept it with undisturbed condition. After that crystal is appeared.

Several strategies have been adopted to prepare polynuclear coordination complexes including the assembly or aggregation of metal centers and ligands, connecting two or several metals with the help of ligand bridges incorporating metal ions into multidentate pockets and bridging ancillary ligand units.

Our aim is to prepare different binucleating ligands to produce some mono, di-, tri- and even polynuclear species. We emphasized on the creation of multinuclear systems with 3d/4d transition metals like Ti, Mn, Fe, Co, Ni, Cu/Zr, Nb, Mo and Y etc. We have also plan to study their single molecule magnetic (SMMs) properties, biological activity (anticancer, antimicrobial, antioxidant) and fluorescent sensing behavior as a function of structural features, nature of metal ions and supporting co-ligands in presence of different N, O donor ligands.

(Separate page may be attached to justify the requirements)

g. Technical Details

- a. TRL
- b. Methodology

Metal complexes will be prepared with stirring for 2-3 hr of synthesized ligand

The salen or ethylenediimine / tetraethylenepentaimmine including 2,6-diformyl-4-methylphenol / salicylaldehyde moiety type of ligands and 1,3,5-tris (4-carboxy phenyl)benzene, 3,5-dinitro benzoic acid, N-(2-hydroxyethyl) iminodiacetic acid and 3,3-dicarboxylic acid-2,2-biquinoline etc with 3d/4d transition metal salts (perchlorate, nitrate, chloride, acetate etc.) in $MeOH$ solution. After completion of reaction precipitated complexes will be collected by filtration, washed with cold $MeOH$ followed by water, and dried under vacuum over P_4O_{10} and then we will try to get single crystals suitable for X-ray analysis with the help of different solvents medium. Prepared complexes will be characterized by CHN analysis, Conductance, UV, IR and NMR spectroscopy. Physical properties and experimental results will further correlated theoretically with the help of DFT.

c. Design & development

Phase-wise plan of action up to post project activities detailing time schedule milestones may clearly be stated.

The 3d/4d transition series metal complexes (acetate, nitrate, chloride, benzoate etc) and perchlorate shall be allowed to react to prepare several new poly-nuclear complexes with different bridging modes of azides, 1,10-phenanthroline and 2,2'-bipyridine etc may be used

as blocking ligands during the preparation. I shall also try to prepare several complexes of (Ti, Mn, Fe, Co, Ni, Cu/Zr, Nb, Mo, Zn, Y) with different ligands like the salen or ethylenediamine / tetraethylenepentaimine including 2,6-diformyl-4-methylphenol / salicylaldehyde moiety type of ligands and 1,3,5-tris (4-carboxy phenyl)benzene, 3,5-dinitro benzoic acid, N-(2-hydroxyethyl) imino-diacetic acid and 3,3-dicarboxylic acid-2,2-biquinoline etc. After the preparation and characterization of these metal complexes, I will try to carry out biological activity (DNA, anticancer, antimicrobial, antioxidant).

d. Facilities and Instrumentation required

- i) Infrared spectroscopy (IR), ii) Nuclear magnetic resonance spectroscopy (NMR, ^1H , ^{13}C) iii) Ultraviolet–visible spectroscopy, iii) A GOUY BALANCE for magnetic susceptibility iv) conductometer, v) X-ray powder diffraction (XRD), vi) PPMS/SQUID for magnetic measurements, vii) Single-crystal X-ray Diffraction.

e. Consumables (Scientific materials)

DETAIL BUDGET FOR PERMANENT EQUIPMENT

(In Rupees)

Sl. No	Estimated cost	Name of equipment*
1.	7000@2 14000/-	Magnetic stirrer
2	6000/-	Heating Mantel
Total: 20 thousand		

BUDGET ESTIMATES: SUMMARY (In Rupees)

Item	BUDGET			
	1st Year	2nd Year	3rd Year	Total
A. Recurring:	NA	NA	NA	NA
1. Remunerations/salaries	3 lacks	3 lacks	2 lacks	8 lacks
2. Consumables	11 thousand	11 thousand	17 thousand	39 thousand
3. Travel	15 thousand	17 thousand	19 thousand	51 thousand
4. Other costs				
B. Non-recurring	15 thousand	NA	NA	15 thousand
Permanent equipment				
Grand Total (A+B)	3.41 lacks	3.28 lacks	2.36lacks	9.05 lacks

h. Expected output and outcome

- The newly design 3d-4f complex clusters will be easily synthesized with low cost reagent availability.
- Investigate with multinuclear systems which have greater oxidizing and reducing power and the neighboring metal ions are expected to „cooperate“ in promoting reactions, electronic magnetic interactions between the metal ions and also have crucial role in deciding the nuclearity and geometry of the molecules.
- Interactions between small molecules and DNA are the primary action mechanism of anticancer activity and designing of molecules that bind and cleave DNA have attracted extensive attention. Transition metal complexes have been widely used to develop synthetic binding and cleavage agents for DNA.

- •The 3d-4f complex clusters may show a large spin state value with a significant anisotropy can behave as single molecule magnets (SMMs).

i. Industry/Institute Collaboration If, yes

- (i) Name of the Collaborating Industry/Institute
- (ii) Collaboration Details
- (iii) Additional Details if any

j. Funding required from I-STEM (with justification):

Details of Requirements&Mode of the Engagement: (Attach the quotation for the consumables)

- (i) Short term Engagement:
 - a. Usage of testing/characterization facilities across the country (Characterization Mode)
 - i. Testing Charges
 - ii. Consumable charges
 - iii. Travel Cost (Boarding and Lodging, if any)
 - b. Usage of fabrication and testing facilities across the country (Fabrication Mode)
 - i. Fabrication and testing Charges
 - ii. Consumable charges (if any)
 - iii. Travel Cost (Boarding and Lodging, if any)
- (ii) Medium term Engagement:
 - a. Execution of project in any one of the Host Institution (Project Mode)
 - a. Fabrication and or testing Charges
 - b. Consumable charges (if any)
 - c. Travel Cost (Boarding and Lodging, if any)
 - b. Execution of project in Multi Host Institutions (Project Mode)
 - a. Fabrication and or testing Charges
 - b. Consumable charges (if any)
 - c. Travel Cost (Boarding and Lodging, if any)

(Round-trip to the Host Institution by 2nd class (Non-AC) railway via the nearest route)

Details of User's Bank Account:

(Please send a copy of the cancelled cheque/copy of the passbook carrying all the information needed)

Beneficiary Name (User's name): Aloke Kumar Ghosh

PAN: BPMPG7993A

Bank Account No.30363286776

Name of the Branch: Kharagpur

IFSC Code: SBIN0000202

Note: Proposed proposal must be executed within stipulated duration (max. 6 month) to avoid fund availability issues. Travel form will be provided by the I-STEM office. The users will submit the technical report, original invoice (duly signed by the Head of the Institution) raised by the Host Institution through I-STEM portal only along with a copy of the travel forms and original tickets through post to the Nodal Officer, I-STEM, Indian Institute of Science, Bangalore. A scan copy of all the documents may be sent in advance.

Dr. Aloke Kumar Ghosh

Aloke Kumar Ghosh

Assistant Professor, Department of Chemistry, Prabhat Kumar College, Contai