Minutes of the meeting of the Departmental Research Project Monitoring Committee (DRPMC) held on 16.01.2024 at 10:00 am in the office of the Dean Faculty of Sciences, University of Jammu, Jammu.

PRESENT:

1. Prof. Anju Bhasin (Convener)
2. Prof. H.N. Sheikh, HOD (HOD Chemistry)
3. Prof. Kamal K. Kapoor (Member)
4. Prof. P.K. Srivastava (Member)
5. Dr. Monika Gupta (Member)
6. Prof. Satya Paul (Special Invitee)
7. Prof. D.S. Sambyal (Special Invitee)

Item No. 1: To consider the progress report of Research & Seed Grant assigned to the following faculty members of the Department of Chemistry:

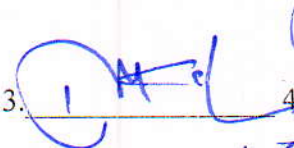
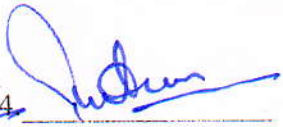
(i) Prof. K.K. Kapoor (Rs. 2.0 lakh)
(ii) Prof. H.N. Sheikh (Rs. 2.0 lakh)
(iii) Dr. Monika Gupta (Rs. 2.0 lakh)
(iv) Dr. Ashwani Kumar (Rs. 2.0 lakh)

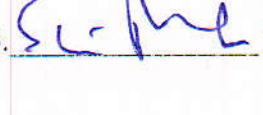
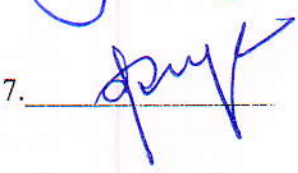
Resolution: The faculty members presented the progress report before the committee members and submitted the hard copy of the same after the discussions and deliberations. The committee members were satisfied with the progress reports of all the projects and appreciated the scientific outcome, especially the sanction of projects by JKSTIC (Prof. K.K. Kapoor, Prof. H.N. Sheikh & Dr. Ashwani Kumar) and submission of SERB-SURE Project to DST, GoI by Dr. Monika Gupta.

Item No. 2: To consider the request of Principal Investigators (PIs) to extend the date of submission of final utilization certificate.

Resolution: The Principal Investigators (PIs) requested to extend the date of submission of final utilization certificate by two months, i.e. March 20, 2024, to enable the PIs to spend the unutilized grant. The DRPMC resolved that the request of PIs be kindly considered for extension by the Dean Research Studies.

The meeting ended with a vote of thanks.

1.  2.  3.  4. 

5.  6.  7. 

Office : 2453969
University : 2435248 } Extension :
: 2435259 } 2617, 2618

Post Graduate Department of Chemistry
University of Jammu
('A+' Grade University- Accredited by NAAC)
Baba Saheb Ambedkar Road, Jammu - 180 006

No. PGD/Chem/

Dated 15-01-2024

NOTICE

Due to unavoidable circumstances, meeting of the Department Research Project Monitoring Committee (DRPMC), scheduled for 15-01-2024 at 4.00 pm, will be held on 16-01-2024 at 10.00 am in the Office of the Dean Faculty of Science to discuss progress report of Research and Seed Grant assigned to following faculty members of the department of Chemistry.

1. Prof. K.K. Kapoor
2. Prof. H.N.Sheikh
3. Dr. Monika Gupta
4. Dr. Ashwani Kumar

The concerned faculty members are requested to submit and present progress report in the meeting

The members of the DRPMC are request to make it convent to attend the meeting.

1. Prof. Anju Bhasin (Convener)
2. Prof. H. N. Sheikh (HOD)
3. Prof. K.K. Kapoor
4. Prof. P.K. Srivastava
5. Dr. Monika Gupta
6. Prof. Satya Paul (Special Invitee)
7. Prof. D.S.Sambyal (Special Invitee)

15-01-2024

Prof. H.N. Sheikh
Head of the Department

Copy to:

Prof. Anju Bhasin Dean Faculty of Science for information please

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University : 2435248 } Extension :
: 2435259 } 2617, 2618

Post Graduate Department of Chemistry
University of Jammu
('A+' Grade University- Accredited by NAAC)
Baba Saheb Ambedkar Road, Jammu - 180 006

No. PGD/Chem/24/ 72-73 Dated 11-01-24.

NOTICE

As desired by Dean Faculty of Science, a meeting of the Department Research Project Monitoring Committee (DRPMC) will be held on 15-01-2024 at 4:00 pm in the Office of the Dean Faculty of Science to discuss progress report of Research and Seed Grant assigned to following faculty members of the department of Chemistry.

1. Prof. K.K. Kapoor
2. Prof. H.N.Sheikh
3. Dr. Monika Gupta
4. Dr. Ashwani Kumar

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1. Prof. Anju Bhasin (Convener)
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5. Dr. Monika Gupta
6. Prof. Satya Paul (Special Invitee)
7. Prof. D.S.Sambyal (Special Invitee)

Prof. H.N. Sheikh
Head of the Department

Copy to:

Prof. Anju Bhasin Dean Faculty of Science for information please

OFFICE OF DEAN RESEARCH STUDIES
UNIVERSITY OF JAMMU

ORDER

Based on the recommendations of the Committee constituted for the purpose vide order No. RA/3977-92 dated 05.12.2022 and also on the recommendations of the Dean of the Faculty concerned, sanction is hereby accorded to the payment of Rs. 2,00,000/- as financial assistance in favour of Prof./Dr. Ashwani Kumar, Department of Chemistry as per the details given below out of the **Research & Seed Grant** for Professor / Associate / Assistant Professor, under the Head **'Quality Assurance Fund (DIQA)'** as per order No. Fin./2022-23/3338-42 dated 16.09.2022:-

a) Hiring of Services / Honorarium for experts	:	-
b) Equipment (Repair) or any accessory, if needed, to the existing equipment	:	50,000/-
c) Purchase of Minor Equipment	:	-
d) AMC's of existing Equipment	:	-
e) Consumables/Chemicals/Glassware etc.	:	1,10,000/-
f) Contingency	:	40,000/-
g) Field work	:	-
h) Any other item		-
Total	:	2,00,000/-

You are required to meet the said expenditure as per University norms. The Principal Investigator (PI) shall submit the bills for pass & payment as per the existing GFR/GeM guidelines to the Grant Section. The quantum of assistance sanctioned is required to be exhausted/utilized within a period of one year starting from the date of issue of order. Utilization certificate will be submitted after completion of the project.

A detailed report of project shall mandatorily be submitted by PI to the office of the Dean Research Studies with a clear statement on whether the said project has enabled the PI to put up a bigger proposal for funding to any national funding agency.

20/1/2023
Assistant Registrar (R&A)

No. RA/23/6086-93
Dated: 20/01/2023

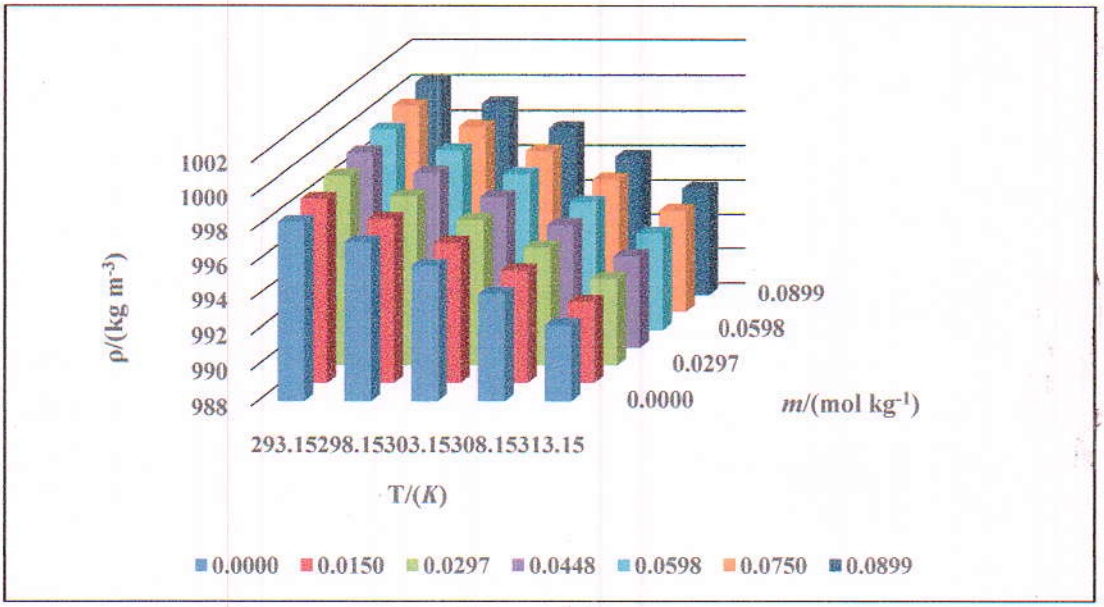
Copy to:

1. Special Secretary to the Hon'ble Vice-Chancellor.
2. Sr. P.A. to DAA/DRS/Registrar/DIQA.
3. Dean of the Faculty concerned.
4. HOD concerned.
5. Principal Investigator.
6. Joint Registrar (Finance).
7. Deputy Registrar (Grants).

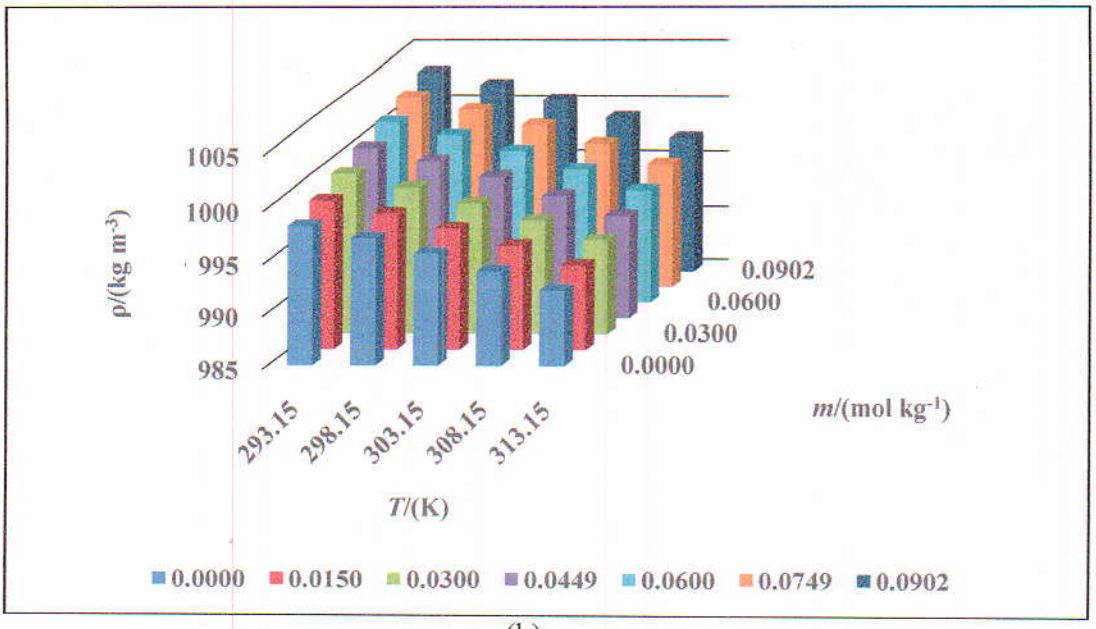
Progress report of the project entitled "**Volumetric, acoustic and viscometric investigations of some protein model components in aqueous solutions of drugs at various temperatures**" supported by **Research & Seed Grant** for Professor/Associate Professor/Assistant Professor of University of Jammu, allocated vide no. RA/23/6086-93 dated 20-01-23, under the Head **Quality Assurance Fund (DIQA)**.

Following are the outcomes of the project:

1. Research Seed money grant assistance helped in the procurement of chemicals for carrying out the preliminary investigations.
2. Density (ρ), ultrasonic speed (u) and viscosity (η) for an essential amino acid and a dipeptide viz. L-leucine and diglycine, respectively in aqueous and (0.0496, 0.1002 and 0.1498) mol kg^{-1} binary aqueous semicarbazide hydrochloride solvent system at five different temperatures ranging (293.15–313.15) K and under barometric pressure have been measured.

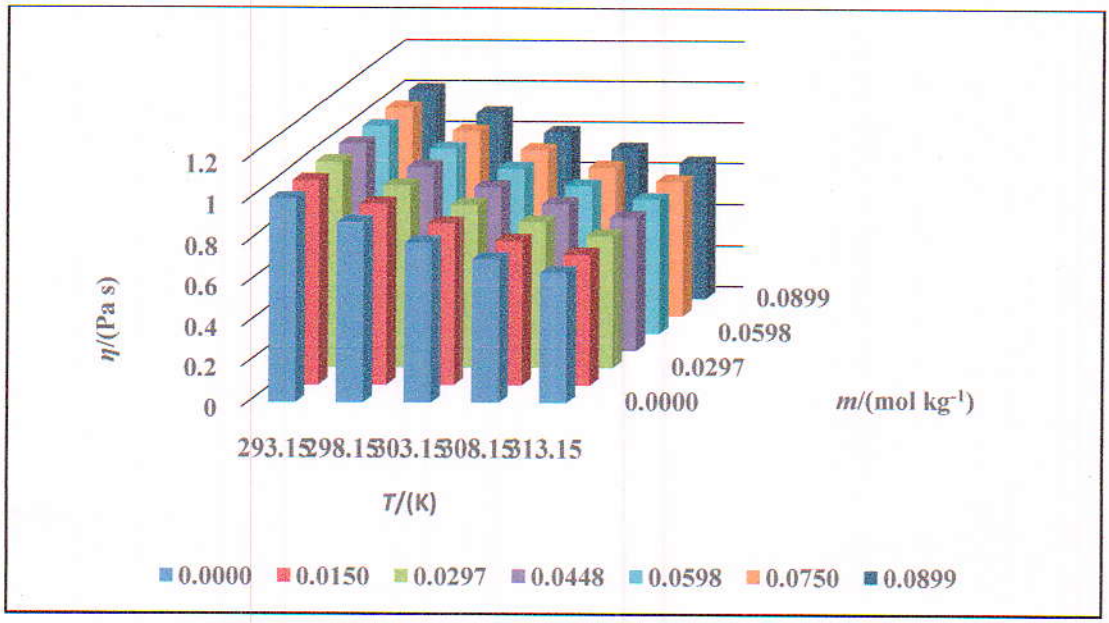


(a)

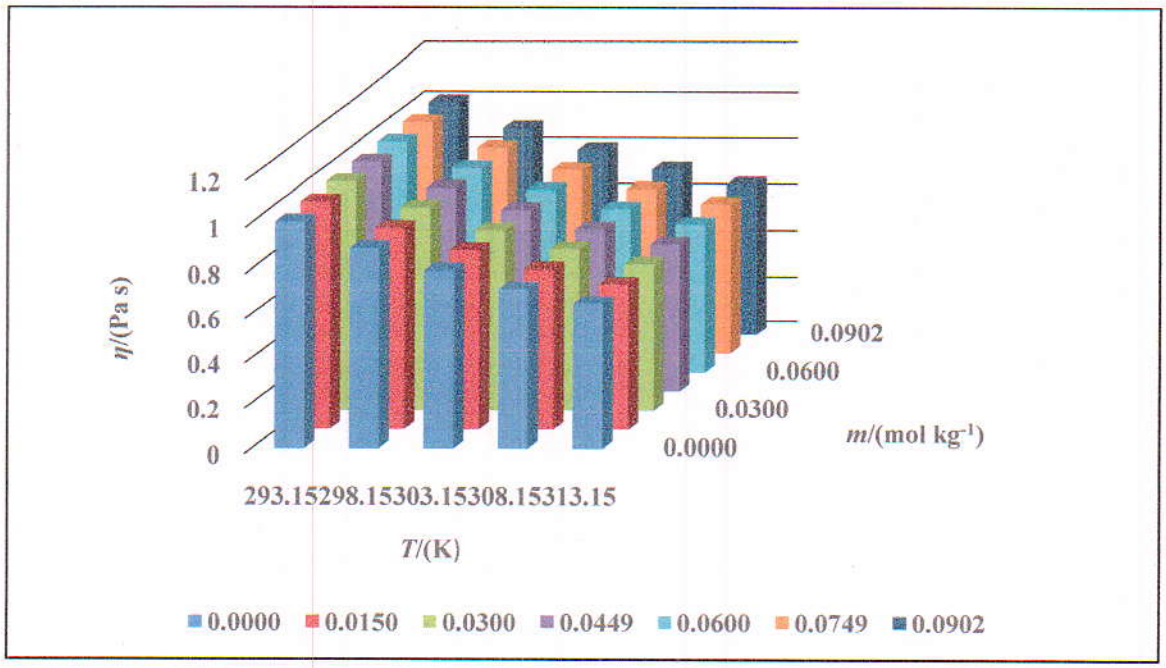


(b)

Fig. 1. 3-dimentional plots depicting alteration of density, ρ with molality and temperature for (a) L-leucine in H_2O, (b) gly-gly in H_2O.



(a)



(b)

Fig. 2. 3-dimentional plots depicting alteration of viscosity, η with molality and temperature for (a) L-leucine in H_2O, (b) gly-gly in H_2O.

3. Varied physicochemical parameters such as apparent molar parameters (V_ϕ, $K_{\phi,s}$), hydration number (n_H), partial molar parameters (V^0_ϕ, $K^0_{\phi,s}$), viscosity coefficients i.e. Falkenhagen and Jones Dole coefficients, transfer parameters etc. have been enumerated from the empirically determined data. Further, the structure breaking character of each examined solute has been scrutinized through the positive sign of temperature derivative of viscosity B-coefficient values and negative sign of $(\partial E^0_\phi/\partial T)_p$ (Hepler's constant) values. In addition, the cosphere overlap model has been utilized for better understanding of various predominant intermolecular interactions in the studied solution systems.

Table 1: Determined partial molar volume, V^0_ϕ, empirical slope, S_v, and calculated partial molar volumes, $\Delta_{tr}V^0_\phi$ for L-leucine and gly-gly in H_2O and mixed aqueous semicarbazide HCl solutions.

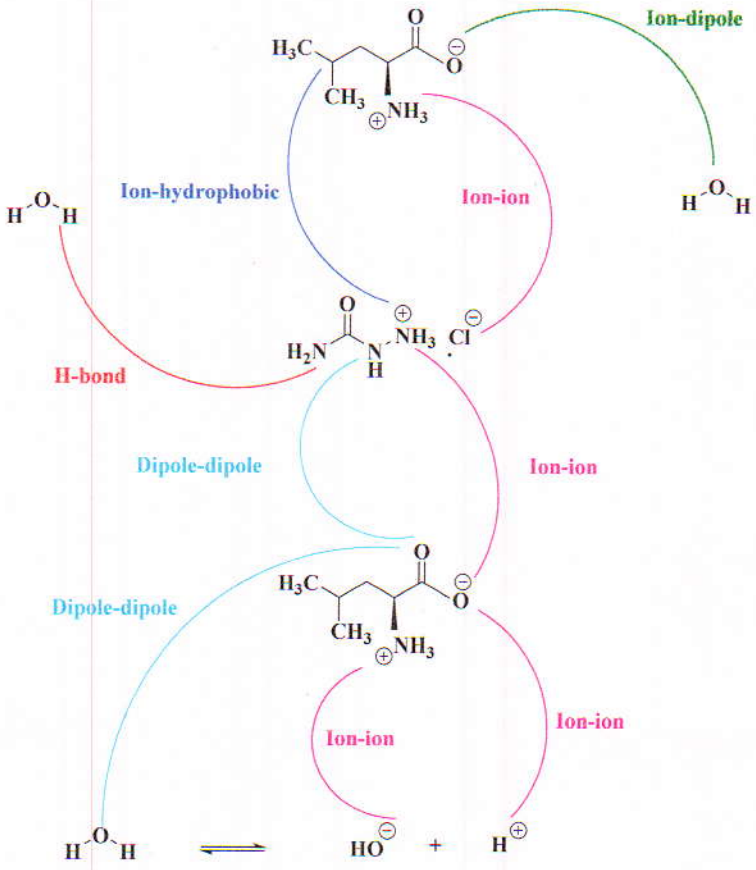
Property	Temperature/(K)				
	293.15	298.15	303.15	308.15	313.15
	L-leucine in 0.0000 *mol kg^{-1} semicarbazide HCl*				
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	107.59 (±0.01)	107.95 (±0.01)	108.34 (±0.01)	108.69 (±0.01)	109.03 (±0.02)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	7.39 (±0.16)	7.39 (±0.08)	7.39 (±0.08)	7.22 (±0.07)	6.88 (±0.28)
	L-leucine in 0.0496 *mol kg^{-1} semicarbazide HCl*				
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	108.18	108.54	108.94	109.29	109.64

	(±0.02)	(±0.01)	(±0.01)	(±0.01)	(±0.01)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	7.28 (±0.34)	7.64 (±0.20)	7.43 (±0.17)	7.43 (±0.17)	7.75 (±0.24)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	0.59	0.59	0.60	0.60	0.61
L-leucine in* 0.1002 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	108.36 (±0.01)	108.73 (±0.01)	109.13 (±0.01)	109.53 (±0.01)	109.88 (±0.01)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	7.91 (±0.15)	7.38 (±0.15)	7.24 (±0.25)	6.98 (±0.11)	6.77 (±0.21)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	0.77	0.78	0.79	0.84	0.85
L-leucine in* 0.1498 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	108.61 (±0.02)	108.98 (±0.01)	109.37 (±0.02)	109.75 (±0.01)	110.10 (±0.02)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	6.25 (±0.37)	6.96 (±0.22)	6.80 (±0.30)	6.86 (±0.18)	7.11 (±0.26)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	1.02	1.03	1.03	1.06	1.07
Gly-gly in* 0.0000 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	75.64 (±0.02)	75.83 (±0.01)	75.96 (±0.02)	76.13 (±0.01)	76.29 (±0.01)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	7.31 (±0.27)	7.04 (±0.24)	7.34 (±0.27)	7.08 (±0.17)	7.44 (±0.25)
Gly-gly in* 0.0496 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	77.27 (±0.03)	77.47 (±0.02)	77.62 (±0.03)	77.82 (±0.02)	77.99 (±0.01)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	8.52 (±0.53)	8.44 (±0.38)	8.71 (±0.47)	8.35 (±0.34)	8.71 (±0.18)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	1.63	1.64	1.66	1.69	1.70
Gly-gly in* 0.1002 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	77.41 (±0.03)	77.61 (±0.01)	77.80 (±0.02)	78.01 (±0.01)	78.19 (±0.02)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	9.36 (±0.39)	9.17 (±0.21)	9.25 (±0.32)	9.25 (±0.18)	9.36 (±0.26)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	1.77	1.78	1.84	1.88	1.90
Gly-gly in* 0.1498 *mol kg^{-1} semicarbazide HCl					
$V^0_\phi \times 10^6/(m^3\ mol^{-1})$	77.48 (±0.02)	77.76 (±0.02)	77.90 (±0.02)	78.13 (±0.02)	78.29 (±0.03)
$S_v \times 10^6/(m^3\ kg\ mol^{-2})$	10.99 (±0.41)	10.21 (±0.26)	10.78 (±0.39)	10.66 (±0.42)	10.87 (±0.44)
$\Delta_{tr}V^0_\phi \times 10^6/(m^3\ mol^{-1})$	1.84	1.93	1.96	2.00	2.00

4. The results acquired from thermophysical explorations of L-leucine and diglycine in pure H_2O and mixed aqueous semicarbazide hydrochloride solvent system have been elucidated depending on varied sorts of intermolecular interactions prevalent in the systems. The outcomes obtained from the enumerated transfer parameters reveal pre-dominance of hydrophilic/hydrophilic and ion/hydrophilic interactions contrary to hydrophobic-hydrophobic interactions. Further, these interactions rise with the progressing temperature and drug's molality owing to

declining electrostriction of each examined solute in the presence of choosen drug. Moreover, the computed hydration number data signifies dehydrating impact of drug on the hydrated solute particles. Furthermore, negative magnitude of Hepler's constant suggests chaotropic nature (structure breaking behaviour) of both L-leucine and dipeptide in the solvent mixtures, which is also supported by positive temperature derivative of Jones Dole coefficient values.

5. Additionally, UV spectroscopic studies have been conducted to understand the existing interactions among drug and protein fragments. Also, the results deduced via volumetric, compressibility and rheological measurements are in agreement with each other.



Scheme: Different intermolecular interactions existing in L-leucine + semicarbazide hydrochloride + water solution.

6. The results of the above systems have been compiled and published in an International Journal namely, "**The Journal of Chemical Thermodynamics, 2024, 188, 107176 (Impact Factor = 2.6)**".
7. Research and seed money grant assistance also helped in preparing a complete research proposal.

The findings of this proposal led to the development of a new proposal which was submitted to the Jammu and Kashmir Science, Technology and Innovation Council (JKSTIC). It is pertinent to mention that this proposal has been awarded with funding of Rs. 7.3 lakh with Serial. No. 8 of the annexure attached (5 pages).

Thanks,

15/1/24

Dr. Ashwani Kumar,

Assistant Professor (Academic Level -12),

PG Department of Chemistry,

University of Jammu,

Jammu.

J. Chem. Thermodynamics 188 (2024) 107176

Contents lists available at ScienceDirect

The Journal of Chemical Thermodynamics

journal homepage: www.journals.elsevier.com/the-journal-of-chemical-thermodynamics

Effect of semicarbazide hydrochloride on the physicochemical properties of L-leucine and glycylglycine at varied temperatures and compositions

Akshita Bandral, Himani Singh, Richu, Qammer Majid, Poonam Rajput, Ashwani Kumar

Department of Chemistry, University of Jammu, Jammu, Jammu and Kashmir 180006, India

ARTICLE INFO

Keywords:
L-leucine
Diglycine
Semicarbazide hydrochloride
Hepler's constant
Cosphere overlap model

ABSTRACT

Density (ρ), sound speed (u) and viscosity (η) for an essential amino acid (L-leucine) and a peptide (diglycine) in water and (0.0496, 0.1002 and 0.1498) mol kg^{-1} mixed aqueous semicarbazide HCl solvent system at five distinct temperatures ranging (293.15 K – 313.15 K) and barometric pressure (101.3 kPa) have been acquired. Varied physicochemical properties like apparent molar parameters ($K_{\phi,S}$, V_{ϕ}), hydration number (n_H), partial molar parameters ($K^0_{\phi,S}$, V^0_{ϕ}), viscosity coefficients i.e. Jones Dole and Falkenhagen coefficients, transfer parameters ($V^o_{\phi,tr}$, $K^o_{\phi,S,tr}$, B_{tr}) etc. have been enumerated from the empirically determined data. Moreover, the structure breaking (chaotropic) character of each examined protein subunit has been scrutinized through positive $\frac{dB}{dT}$ (temperature dependence of viscosity B-coefficient) values and negative $(\partial E^O_\phi/\partial T)_p$ (Hepler's constant) values. In addition, the cosphere overlap model has been used for a better understanding of assorted predominant molecular interactions in the examined solution mixtures.

1. Introduction

Protein (polymer of amino acids) constitutes a major group of biological macromolecules that are vital for the functioning of a living system. It has a significant physiological function and an imperative role in the maintenance of body tissues, including development and repair. It is the chief source of energy and is implicated in the synthesis of hormones, prevents infections, controls different body functions and produces enzymes which accelerate different chemical reactions occurring inside the body [1]. The thermophysical explorations on protein fragments i.e. amino acids, peptides and their derivatives in different solvent media have led to a remarkable deal of interest as explorations on these fundamental building blocks of life furnish better insights into the effect of different additives such as drugs, surfactants, vitamins, salts etc. on biomolecules [2–4]. Further, these investigations also provide useful data for interpreting hydration characteristics and different sorts of interactions that are prevalent in varied biochemical and physiological processes. Due to the complicated molecular arrangements, it is hard to directly analyse the protein interactions. Hence, different model compounds of proteins that imitate some definite characteristics of protein structure in aqueous solutions are usually investigated [5–7]. On the other hand, drugs play a key role in human health and livestock rearing. Various thermodynamical, structural and biological explorations play significant task in comprehending the pharmacological action of drugs which is necessary for their discovery, designing and activity at the molecular level. Further, the pharmacodynamics and pharmacokinetics of the drug are considered as the outcome of various physicochemical interactions among drug and functionally imperative substances in the living being [8–10]. Moreover, the drug that enters the body tends to stimulate certain ion channels, receptors, act on transporter proteins or enzymes, leading to specific reactions/biochemical processes in the body and interact by binding at specific sites with the receptors. Once activated, the receptor stimulates a specific response either directly in the body or by causing the release of hormone or/and other endogenous drugs in the body. As most receptors are usually proteins, drugs can interact with amino acids/peptides to modify the conformation of the receptor proteins. Hence, it is of considerable interest to explore the interactions amongst model compounds (amino acids/peptides) and drug molecules in order to understand its action in the body.

Therefore, in this work we have carried out thermophysical explorations on L-leucine and gly-gly in aqueous and binary aqueous mixtures of semicarbazide hydrochloride at distinct temperatures. L-leucine (essential amino acid) is used in the synthesis of proteins and is vital for muscle build-up and repair. Further, it helps to regulate blood sugar levels and energy, produces growth hormones, improves immunity, wound healing and also benefits endurance performance [11]. Whereas,

* Corresponding author.
E-mail address: [redacted] (A. Kumar).

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Available online 9 September 2023

(Rs. In lakhs)

SPONSORED RESEARCH AND EXTENSION-2022-23

University of Jammu

Name of Principal Investigator with Contact Details E-mail /cell No.	DOB/DOR	Subject/Field	Title of the Project Proposal	Institution / Organization	Funds Proposed by the Technical Committee			Remarks
					1st Year	2nd Year	Total	
2	3	4	5	6	10	11	12	13
Prof. Seema Langer, Dean Life Sciences, Professor & Head, langerseema@yahoo.co.in 9906027016	05-06-1964	Zoology	Investigations on nutritional and clinical significance of fresh water crabs with special emphasis on the effect of frozen storage on their biochemical composition	Department of Zoology, University of Jammu	3.75	2.75	6.50	Recommended
Dr. Sikander Pal, Associate Professor, sikandersb@jammuuniversity.in, sikanderchowdhary@gmail.com 9596744900	27-04-1981	Botany	Genome wide association studies (GWAS) of maize roots for improving traits regulating phosphate use efficiency	Department of Botany, University of Jammu	4.50	3.50	8.00	Recommended
Dr. Nirmala Sharma, Professor, nsharmabot@gmail.com 9086003468, 7006275841	17-03-1965	Botany	Exploration of variability in genetic systems of Artemisia species abounding NW Himalayas with emphasis on the economic and evolutionary significance of chromosomal races.	Department of Botany, University of Jammu	4.00	3.00	7.00	Recommended

	Veenu Kaul, Professor, veenukaul@yahoo.co.in 9419137180	08-12-1969	Botany	Evaluation of cytological molecular and biochemical diversity in Drimia indica (Roxb.)Jessop.	Department of Botany, University of Jammu	4.00	4.00	8.00	Recommended
5	D. S Bharathiraja, Assistant Professor, bharu.ap@gmail.com 9543453909		Biotechnology	Surface fabrication of Biopolymer Scaffolds with Nano Hydroxyapatite and extracts of Aegle Msarmelos and/or Catharanthus Roseus for boneRegeneration : An IN-Vitro study.	School of Biotechnology, University of Jammu	4.10	3.75	7.85	Recommended
6	Dr.Madhulika Bhagat, Associate Professor Madhulikasbt@gmail.com 9419174018	09-04-1979	Biotechnology	Development of polymeric nanogels loaded with essential oil from medicinal and aromatic plants.	School of Biotechnology, University of Jamrau	4.50	3.00	7.50	Recommended
7	Prof. Haq Nawaz Sheikh, Professor, nn.sheikh@jammuuniversity.ac.in nnsheikh07@gmail.com hnsheikh@rediffmail.com 7006282851, 9419148797	23-08-1969	Chemistry	Development of Luminescent Lanthanide-Coordination Polymers/Metal organic Frameworks as Chemical Sensors.	Department of Chemistry, University of Jammu	4.50	3.70	8.20	Recommended
8	Dr.Ashwani Kumar, Senior Assistant Professor, ashwani.kalsi@gmail.com 9419860841, 9596895135	17-05-1986	Chemistry	Temperature dependent physicochemical studies of citrates/tartrates in aqueous solutions of ionic liquids.	Department of Chemistry, University of Jammu	4.00	3.30	7.30	Recommended

	Shd Sarfaraz Asgher, Associate Professor, sasgher20@gmail.com sarfarazasgher@jammuuniversity.ac.in 09419134864, 0191-2439279	10-12-1974	Geography	Assessment of climate change on the sustainability of wetlands in Jammu Division	Department of Geography, University of Jammu	3.00	3.00	6.00	Recommended
20	Dr.Shashi Prabha Assistant Professor, sprabhe[illegible]gmail.com 9419106[illegible]		Geography	Variability Analysis of Climate change for sustainable Agriculture: An Agro-Ecological based approach of the Himalayan and Sub-Himalayan regions of Union Territory of Jammu & Kashmir.	Department of Geography, University of Jammu	3.00	3.00	6.00	Recommended
21	Dr. Ashok Kumar, Assistant Professor, ashoksharma@jammuuniversity.ac.in 9419106800	25-12-1977	Computer Science/IT	Designing a Predictive model for Analyzing the Academic performance of Learner's in Higher Education in UT of Jammu and Kashmir by using Artifical Intelligence approaches.	Department of Computer Science & IT, Bhaderwah Campus University of Jammu	3.00	1.75	5.75	Recommended
22	Dr.Jatinder Manhas, Sr.Assistant Professor & Head, jatindermanhas@jammuuniversity.ac.in 8082770939, 9419173793	21-03-1980	Computer Science/IT	Artificial Intelligence based landslide Monitoring and Forecasting System in the UT of Jammu & Kashmir.	Department of Computer Science & IT, Bhaderwah Campus University of Jammu	4.30	2.70	7.00	Recommended
					Total :	91.40	71.20	162.60	

Utilization of Research & Seed Grant under DIQA

S.No.	Heads	Amount Sanctioned	Utilized	Unutilized
1	Consumables	1,10,000/-	1,09,760/-	240/-
2	Equipment (Repair) or any Accessory	50,000/-	49,991/-	9/-
3	Contingency	40,000/-	39,972/-	28/-
	Total	**2,00,000/-**	**1,99,723/-**	**277/-**