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1. A series of memantine based salts with various aromatic and aliphatic carboxylic acids: Crystallographic analysis, Hirshfeld surfaces and dissolution study
   **Varsha Bhardwaj**, Mayuri Shaiwale, Bhamini Lakhani, Amar Ballabh*, *Journal of Molecular Structure* 1206 (2020) 127672.
2. Design, synthesis, and application of a new series of organogelator using crystal engineering approach and solvent parameter study: A synergetic approach
   **Varsha Bhardwaj**, Amar Ballabh*, *Journal of Molecular Liquids* 322 (2020) 114520.
3. A series of multifunctional pivalamide based Low Molecular Mass Gelators (LMOGs) with potential applications in oil-spill remediation and toxic dye removal
   **Varsha Bhardwaj**, Amar Ballabh*, *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 632 (2022) 127813.
4. Design and synthesis of novel heterocyclic pivalamide ligands and their copper(II) complexes: Structure, BSA/DNA interactions and SOD *synzyme* activity
   **Varsha Bhardwaj**, Priyanka S. Salunke, Aditya A. Puranik, Neelima D. Kulkarni*, Amar Ballabh*, *Polyhedron* 225 (2022) 116054.
5. Remediation of Marine Oil Spills and Water Pollution using Low Molecular Weight Organo-Gelators (Perspective)
   **Varsha Bhardwaj***, Amar Ballabh*, *Recent Advances in Petrochemical Science* 7 (2022) 1-3.
6. Chapter 2 – Multifunctional Supramolecular Gels – An Overview. in *Advances in Chemistry Research. Vol. 76* (Nova Science Publishers, USA, 2022)
   **Varsha Bhardwaj**, Amar Ballabh*.
7. Chapter 5 – Low Molecular Mass Gelators Based on Thiazole Derivatives – Design and Function. in *Advances in Chemistry Research. Vol. 76* (Nova Science Publishers, USA, 2022)
   **Varsha Bhardwaj**, Amar Ballabh*.

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# A series of memantine based salts with various aromatic and aliphatic carboxylic acids: Crystallographic analysis, Hirshfeld surfaces and dissolution study

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ABSTRACT

Memantine.HCl (MEM.HCl), an adamantane based amine is a clinically useful drug for the treatment of various neurological disorders. Surprisingly, applications of MEM salts/cocrystals in crystal engineering, as a supramolecular motif, are rarely reported in literature, in spite of opportunity that MEM salts (primary ammonium monocarboxylate, PAM and primary ammonium dicarboxylate, PAD) provide to study the reliability and stability of various non-bonded interactions such as C—H···O, C—H···N, van der Waals, etc. in presence of strong ionic hydrogen bonds ($N^+$ —H…$O^-$, O—H··· O, etc.). In the present study, a new series of 12 salts with MEM and varied carboxylic acid backbones (aliphatic and aromatic) were synthesized and characterized by various physicochemical techniques such as IR, NMR and single crystal X-ray studies. The focus was also directed to understand the supramolecular synthons present in these salts and establish a structure-property relationship among them. Qualitative (graph set analysis) and quantitative (Hirshfeld surface analyses) approaches were also employed to analyse all the single crystal structures of salts (**1A**-**1K**) to gain an insight regarding the supramolecular assemblies formed and some subtle variation in the well-established PAM and PAD supramolecular synthons. Additionally, all the synthesized salts were subjected to solubility studies in water and compared with the standard MEM. HCl salt. All synthesized salts displayed a range of solubility in water from high to medium to low as compared with MEM. HCl salt. Efforts were also directed to understand the possible cause of high and low solubility of newly synthesized MEM salts in water with respect to the carboxylic acid backbone, ratio of acid/amine (present in salts) and the supramolecular synthons present in the single crystal structures. Moreover, supramolecular isomerism of 1D PAM to 0D PAM, with bulky group substituted carboxylic acid (pivalic acid and 4-methylbenzoic acid), suggests bright future prospects of designing new materials from crystal engineering point of view.

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## 1. Introduction

Over the years, crystal engineering [1—3] has emerged as one of the fastest growing areas in research because of its applications in drugs and pharmaceuticals (polymorphs, pseudo-polymorphs), organic electronics, optical devices, molecular machinery, and many more [3,4]. The field of crystal engineering (or solid-state supramolecular synthesis) deals with the understanding of intermolecular and intramolecular interactions (present in a structure) in the context of crystal packing and applying the understanding to design the pre-desired crystal structures with specific physical or chemical properties [5]. In the recent years, transformation of APIs from their original form into co-crystals has gained a lot of interest. A salt/co-crystal of an API is expected to show modified physical and chemical properties than the pure compounds, which enables us to improve the bioavailability of the drug, thus creating an attractive route for drug development [6]. As a result, crystal engineering approach proved to be quite fruitful in modifying the properties of drugs, viz. solubility, dissolution rate, bioavailability, melting point, stability and compressibility [7—19].

We have been working in the area of design, synthesis and application of new Low Molecular mass Gelators (LMOGs) [20,21], using crystal engineering approach, since a decade. Recently, we got interested in physicochemical alteration of a known drug

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# Design, synthesis, and application of a new series of organogelator using crystal engineering approach and solvent parameter study: A synergetic approach

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ABSTRACT

A new series of organic salts (**A1B1-A1B6**) based on pivalic acid and primary amine (alicyclic, aromatic, aliphatic) has been designed and synthesized for its potential organogelation behavior. A simple strategy of synthesizing 1-D hydrogen bonded network of PAM (primary ammonium monocarboxylate) leads to the discovery of five new gelators. All the synthesized salts (gelator/non-gelator) were subjected to single crystal X-ray studies to support the hypothesis that 1-D hydrogen bonded networks favor gelation. A detailed study of solvent parameters like dielectric constants, Kamlet-Taft parameters, Hansen parameters, etc. was carried out to get an insight into the role of solvents on the thermal stability and gelation performance of these salts. Organogelation behavior of Salts (**A1B1-A1B5**) is found to be dependent upon bulk solvent properties such as dielectric constant ($\varepsilon$), polarity index ($P'$) and a strong correlation between multi-component solvent parameters such as ($\beta$) and polar cohesive energy ($\delta_p$) is observed. Gel network of salt **A1B3** (in Acetonitrile solvent) has been used as a template for synthesis of silver nano particles owing to its rectangular hollow xerogel fibers.

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## 1. Introduction

'Supramolecular gel', a non-covalently bonded colloidal system, contains nano-scale molecular assembly of solutes capable of immobilizing solvents [1–4]. Supramolecular gels are invariably correlated with low molecular weight organo gelators (LMOGs) comprising of small (molecular weight <3000) compounds, which can form self-assembled fibrilar networks (SAFiNs) through various non-covalent interactions such as hydrogen bonding, van der Waals interaction, π-π interaction, hydrophobic interactions, etc. resulting in the gelation of solvent (aqueous/organic). Last decades have seen an enormous rise in the research revolving around thermo-reversible multicomponent LMOGs owing to their innumerable applications like templating agents, smart materials, optoelectronic materials, pollutant removal, reusable catalysts, to name a few [5–7].

Multicomponent supramolecular gelators [8–10], a member of the vast family of LMOGs, represent a special position in the ever-growing list of compounds displaying gelation properties, mainly due to: (i) simplicity of the system to understand the mechanism of gelation, especially, when the number of non-bonded contacts are limited (ii) multiple functionalities can be envisaged in a single system by suitable choice of individual components and (iii) crystal engineering approach can be applied successfully to design a new two-component gelator.

In recent years, crystal engineering has been proved to be an inevitable tool for designing new gelators, using the concept of supramolecular synthons [11,12]. Crystal engineering strategy can help us to design a molecule with a preferential 1-D hydrogen bonding network, a prerequisite for supramolecular gelation. Understandably, the anisotropic growth of molecular assemblies results in the formation of a continuous network of ribbons, fibers, rods, tubes, etc. [13–15] which further entangle among themselves through weak non-covalent interactions forming a three-dimensional network, thereby trapping bulk solvents, as a result of capillary forces and surface tension.

Inspired by our recent success with organic salts, namely 2-aminothiazole containing salts [16] (supramolecular gelation study) and memantine based salts [17] (crystal engineering study), we decided to work with simple two-component systems possessing the potential to show supramolecular gelation. Surprisingly, a simple acid molecule of tert-butyl carboxylic acid (pivalic acid), which lacks long aliphatic chain, but has multiple methyl groups that can induce steric hindrance and may contribute to various weak non-bonded interactions such as C-H…O, C-H…N, C-H…π, etc. has never been considered for supramolecular gelation studies. However, few pivalic acid salts have been reported in the literature due to its interesting hydrogen bonded network, and surprisingly, their gelation property was never explored [18].

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# A series of multifunctional pivalamide based Low Molecular Mass Gelators (LMOGs) with potential applications in oil-spill remediation and toxic dye removal

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## ABSTRACT

Designing new Low molecular weight gelators (LMOGs) which can congeal organic/aqueous solvents is a daunting task, especially those capable of selective organogelation in presence of oil/water systems. Phase selective organogelation (PSOG) offers various advantages over conventional methods for oil spill remediation, viz. programmability, responsiveness and biocompatibility. Molecules with multiple fragments such as one-dimensional hydrogen bonding groups, terminal bulky group and a variable organic moiety (aromatic, aliphatic, alicyclic) appear to be good candidates for design of new LMOGs. In this work, a new series of pivalic acid based amides (**1A–13A**) having aromatic, aliphatic and alicyclic backbones were synthesized and characterized by various physicochemical methods. All the compounds were exploited for their ability to congeal various organic solvents including crude oil fractions, fuels and oils. Out of 13 newly synthesized compounds, six turned out to be excellent organogelators. Multifunctional properties of these compounds were observed such as selective gelation of aliphatic solvents in presence of water and removal of dyes from aqueous medium with good efficiencies. A detailed study is undertaken to establish the cause of gelation/non-gelation of solvents based on structure-property correlation using single-crystal X-ray diffraction, powder X-ray diffraction, Hirshfeld surface analysis, etc. Moreover, these compounds represent a class of one of the smallest molecules explored for the application of phase selective organogelation of fuel for containing oil-spills and dye adsorbing materials for water pollution control.

*Abbreviations:* PSOG, phase selective organo-gelation; MGC, minimum gelator concentration; LMOG, low molecular weight organo-gelator.

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# Design and synthesis of novel heterocyclic pivalamide ligands and their copper(II) complexes: Structure, BSA/DNA interactions and SOD *synzyme* activity

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ABSTRACT

Four new heterocyclic pivalamide based ligands (**L1-L4**) and their respective mononuclear copper(II) complexes (**C1** = [Cu(N-(thiazol-2-yl)pivalamide)$_2$], **C2** = [Cu(N-(5-methylthiazol-2-yl)pivalamide)$_2$], **C3** = [Cu(N-(benzothiazol-2-yl)pivalamide)$_2$], **C4** = [Cu(N-(benzoimidazol-2-yl)pivalamide)$_2$]) were synthesized to serve as low molecular weight SOD mimics. The complexes were characterized by single crystal XRD, Hirshfeld surface analysis, FT-IR, UV–vis, EPR and ESI-MS studies. **C1** crystallizes out in a triclinic system with P-1 space group, while **C2** and **C4** belong to P2$_1$/*c* and P2$_1$/*n* space groups respectively, from monoclinic system. The crystal structures indicate nearly square planar geometry where mononuclear copper(II) metal ions have coordinated with O and N donor atoms of the pivalamide ligands in *trans* fashion. All the complexes can scavenge superoxide concentration at low concentrations, in the order **C2** < **C3** < **C1** < **C4**. The interaction of all the complexes with BSA (bovine serum albumin) protein investigated using fluorescence titration method indicated a static quenching mechanism ($K_{BSA}$ values of the order $10^5$ $M^{-1}$). The ability of the complexes to bind with calf thymus DNA were also evaluated using absorption and fluorescence titration methods and an intercalative interaction mode of the complexes with DNA was established ($K_b$ values of the order $10^4$ $M^{-1}$). The complexes have a strong ability to cleave supercoiled plasmid DNA.

## 1. Introduction

Supramolecular chemistry is the study of non-covalent interactions in organic solids, metal complexes and organometallic compounds. In coordination chemistry, the binding of bioactive molecules to their bioactive targets occurs primarily through supramolecular interactions. With decades of dedicated work in the design and synthesis of novel supramolecular architectures, supramolecular synthesis of multi-functional systems has evolved and brought us closer to develop such systems for the betterment of mankind. The key is to gain control over supramolecular assemblies, which can contribute to development of host–guest assemblies, target selective drug delivery, biosensors, tissue engineering, etc. [1].

Thiazole containing compounds are widely known for their exclusive biological properties like anti-protozoal, anti-convulsant, anti-diabetic, anti-inflammatory, anti-tumor, antiviral, and many more because of the presence of –N═C–S– group. Thiazole based metal complexes have been widely studied in the past for their promising anti-fungal, anti-bacterial and cytotoxic behavior [2–5]. This inspired us to investigate the properties of synthesized complexes for their newer biological activities.

Redox-active transition metal ions in a coordination environment make good candidates for biological catalytic activity in redox reactions [6,7]. Specially, copper(II) containing coordination complexes possess redox potentials similar to those of reactive oxygen species, and hence, can be best utilized in catalyzing the dismutation of superoxide anion (a product of oxygen metabolism in the living systems). This superoxide ion can be a mediator of reperfusion diseases such as myocardial infarction (stroke), initiate inflammatory processes associated with diseases like arthritis, even cause oxidative injury to the tissues which can lead to various neurological disorders like Parkinson's and Alzheimer's [8]. Naturally occurring superoxide dismutases (SOD) in living

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# Remediation of Marine Oil Spills and Water Pollution using Low Molecular Weight Organo-Gelators

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**Abstract**

Low molecular weight organo-gelators (LMOGs) can be employed for efficient removal of oil, toxic dyes, metal ions as well as organic pollutants from water bodies. An effective self-assembly assisted by non-covalent interactions holds the key to formation of a three-dimensional network capable of immobilizing the oil phase. The authors here present a personal perspective on the basic understanding and credibility of such gelation systems.

**Keywords:** Organo-gelators; Oil spills; Water pollution; Biocompatibility; Futuristic aspects; Organo gel

**Abbreviations:** LMOGs: Low Molecular Weight Organo-Gelators, PSOG: Phase Selective Organo-Gelation

## Introduction

Molecular gels are self-assembled systems where the solute molecules (gelators) interact and combine via various non-covalent interactions such as H-bonding, van der Waals forces, π-π bonds, hydrophobic interactions, charge transfer, etc. and form one dimensional fibers, which on aggregation, form 3D assemblies which can trap a solvent, forming a gel. Gels are visco-elastic materials [1-3] which display flow characteristic on application of strain. And as the saying goes, if you wish to identify if a given substance is a gel or not, well, "If it looks like Jell-O, it's a gel…" [4] Gels can defy gravity and an inverted vial containing a gel will likely resist its ability to flow. The underlying principle seems very simple, yet it gets complex as we dig in deeper. Since it depends on a variety of factors whether a particular molecule will congeal a particular solvent or not, most of the gelators have been discovered by serendipity and not by design. The mechanism at molecular level is not even fully understood till today. As was rightly quoted by D. J. Lloyd, "the colloid condition, the gel, is easier to recognize than to define" [5].

Gels are broadly classified based on solvents gelled by them; hydrogels, where the solvent being gelled is water and organo gels, where organic solvents are involved. The gelator molecules can belong to various classes like polymers, multi-component systems, small molecules, peptides and many more! They are employed for various high-tech applications in molecular sensing, energy storage, catalysis, tissue engineering, drug delivery, templating, cosmetics, dyes, adhesives, thickening agents, and many more [6]. They also have a great potential to be used as smart materials as they are highly versatile systems which can respond to light, heat, ultrasound waves, pH, etc. They inevitably stand out because of their indispensability, biocompatibility, and programmability.

## LMOGs for Tackling Oil Spills

Marine oil spills are the result of natural or accidental discharge of crude oil and petrochemicals in the water bodies. In April 2010, the Deepwater Horizon oil rig suffered an explosion in the Gulf of Mexico and leaked millions of barrels of crude oil in the ocean. This, however, was not the first report of marine oil spill. According to statistics, more than a thousand oil spills are reported every year. While they are not necessarily as dreadful as the Deepwater Horizon, they still cause long-term damage and pose serious threat to marine ecosystem. The consequences can be disastrous, which contribute to environmental pollution, severely affected marine flora and fauna, spillage of non-renewable fossil

**James C. Taylor**
Editor

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## Chapter 2

# Multifunctional Supramolecular Gels – An Overview

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## Abstract

Supramolecular gels belong to the class of soft materials, which can display both, solid- and liquid-like properties under the influence of external mechanical stress. They are typically dilute systems containing a very small amount of Low Molecular Weight Gelator (LMWG) which can self-assemble into nano-scale network causing the solvent phase to immobilize, forming a gel. This happens as a result of a combination of complementary supramolecular interactions such as electrostatic, hydrophobic, van der Waals, hydrogen bonding, π-π, etc. to generate hierarchically ordered supermolecules. Molecular gels are highly functional materials which can respond to external stimuli like heat, light, ultrasound, change in pH, presence of redox-active species, ions, enzymes, applied voltage, magnetic field, etc. In this chapter, we intend to discuss the various applications of low molecular weight gelators which highlight their key advantages like exquisite tunability, self-healing ability, self-programmability and certain aspects which can guide our way to design such functional materials *a priori*, which has so far, remained a challenging task. We have tried to summarize the recent advancements in terms of the widespread applications they offer owing to their exclusive physical and chemical properties.

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## Chapter 5

# Low Molecular Mass Gelators Based on Thiazole Derivatives: Design and Function

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## Abstract

In the recent years, advancements in supramolecular chemistry have brought us closer to the designing of low molecular weight gelators with desired properties and advanced applications. In that regard, thiazole-based gelators comprise a unique class as they are extremely versatile in terms of molecular design and offer wide range of applications, like template directed synthesis of desired nano structures, selective sensing of ions, heavy metal gelation, specialized polymerization, and many more. Besides, thiazole-based compounds are well-known for their anti-bacterial, anti-cancer and anti-inflammatory properties, which offers an edge in terms of biological applications. The concept of crystal engineering can also be employed to study the interactions and supramolecular assemblies formed by these systems, which can bring us closer to understand the peculiar mechanism of gelation and formation of SAFiNs (self-assembled fibrillar networks). In this chapter, we focus on various supramolecular assemblies formed by simple thiazole derivatives to establish structure-property correlation and their futuristic aspects.

**Keywords:** low molecular weight-gelators, supramolecular assemblies, crystal engineering, self-assembled fibrillar networks, structure-property correlation

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# *Papers Presented*

1. 45th National Seminar on Crystallography (NSC 45), IIT-BHU (Varanasi), July 9-12, 2017; entitled **Design, Syntheses and Single Crystal Studies of Memantine based Salts.**
2. Research meet held at IIT-Gandhinagar by Indian Society of Radiation and Photochemical Sciences, August 19, 2017; entitled **Supramolecular assemblies of a pharmaceutically important drug and its salts: A Crystal Engineering approach.**
3. International conference on Emerging trends in Chemical Sciences (ETCS-2018, Dibrugarh, Assam), February 26-28, 2018; entitled **Investigation of Hydrogen bonded Supramolecular networks in cocrystals/salts of Adamantane based API.**
4. One day National Seminar on Decadal Trends in Chemistry Research: The perspective of Women Scientists – WCHEM 2020 (Vadodara), March 8, 2020; entitled **Crystal Engineering approach to a new class of Two-component Organo-gelators.**
5. International Conference on Recent Trends in Chemical Sciences (RTCS-2021) organized by Indian Chemical Society, Kolkata; December 21-24, 2021; entitled **'A series of low molecular weight organogelators (LMOGs) with potential applications in phase selective organogelation (PSOG) at room temperature-possible implementations in oil spill remediation and toxic dye removal studies'** (*Oral Presentation*) – Awarded with **Professor Santi Ranjan Palit Memorial (Young Scientist) Award**.

# Conferences and Workshops

1. Science Conclave – MSU Baroda; 28 February 2017.
2. ECell 2k18-19 Cheminformatics Workshop – MSU Baroda; 16-17 February 2019.
3. Applications of X-ray Techniques - XRF, XPS, Auger – MSU Baroda; March 9, 2019.
4. Green Conference on 'Save Mother Earth'– MSU Baroda; October 10, 2019.
5. DST & ACS Workshop: CSMCRI Bhavnagar; November 15, 2019.
6. Advanced Analytical Techniques for Elemental Analysis (AAT-2019) – MSU Baroda; December 28, 2019.
7. Science Conclave – MSU Baroda; February 28, 2020.
8. Workshop on Computational Chemistry (CCW-2020) – MSU Baroda; March 3-7, 2020.
9. Rigaku School for Practical Crystallography – A Rigaku Event; June 1-5, 8-12, 2020.
10. One Day National Symposium on Frontiers in Chemistry and Medicinal Chemistry (FICM-2021) – MSU Baroda; October 11, 2021.
11. National Symposium on Frontiers in Chemistry (NSFC-2022) – MSU Baroda; June 25, 2022.

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