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PROGRAM BOOK

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Keynote Lecture (Room207)

August 23 16:20-17:00 (Room207) Chairman: Prof. Masato Ito

Functionality design of heteroaromatic compounds

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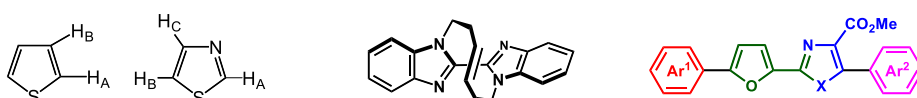
Key words: heteroaromatic compound; transition metal catalysis; C–H coupling; photoluminescence; biomass

Heteroaromatic compounds show remarkable properties in organic chemistry. A number of molecules bearing heteroaromatic rings are employed for the purpose of pharmaceutical and agrochemical drugs exhibiting biological activities. Those have also been shown to be available as advanced materials when the oligomers and polymers of heteroaromatic compounds constitute extended π -conjugation. We herein describe synthesis of several heteroaromatic compounds in our group applying transition metal catalysis.

Bond formation at the C–H bond of five-membered heteroaromatic compounds such as thiophene and thiazole smoothly proceeds in the presence of nickel and palladium catalysts. The reaction with various organic halide gives the coupling product with extended π -conjugation. Several molecules were shown to exhibit photoluminescence and whose efficiencies and wavelengths were tunable based on the electronic effect of the substituent. The reaction of 2-halo-3-substituted thiophene with a strong base representative as bulky magnesium amide such as 2,2,6,6-tetramethylmagnesium chloride (lithium chloride salt) $\text{TMPMgCl}\cdot\text{LiCl}$ underwent deprotonation at the C–H bond of the thiophene ring. Following addition of a nickel catalyst induced cross-coupling polymerization leading to highly regioregular head-to-tail-type poly(3-substituted thiophene) with controlled molecular weight and the molecular weight distribution.

Homocoupling of heteroaromatic compounds at the C–H bond leads to the dimerized product. Modification of the structure of the thus obtained heterobiaryl leads to a compound bearing molecular asymmetry, which induces chirality without possessing a carbogenic chiral center. We named such heterobiaryls as 'winding vine-shaped molecular asymmetry' and these compounds were shown to be separated by HPLC with a chiral column and/or produced by asymmetric synthesis using a chiral catalyst. Properties and functionalities of such vine-shaped compounds are studied.

The C–H coupling of heteroaromatic compounds is also available for furan derivatives, which are composed of five-membered heteroaromatics containing oxygen. C–H coupling of furan with several aromatic halides leads to a variety of compounds involving extended π -conjugation and these molecules showed photoluminescent characteristics, which are potentially applicable to electroluminescence (EL)/light emitting diodes (LED). Condensation of diols and diamines with dimerized furan carboxylates afforded the corresponding polyesters and polyamides. Since furfural a furan derivative is produced by the degradation of biomass cellulose followed by acid treatment, the obtained polyesters and polyamides can be recognized as bioplastics.



Oral Presentation (Room207)

1-OP 9:50

August 23 (Room207)

Chairman: Prof. Guan-Yeow Yeap

Research Activities at Physical Chemistry Section

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Key words: Physical chemistry; molecular modelling; green chemistry; environmental science; surface science

ABSTRACT

The School of Chemical Sciences was established in 1969 and is divided into Organic, Inorganic, Physical, Analytical and Industrial Chemistry sections. The school offers two undergraduate programmes namely Bachelor of Science in Pure Chemistry and Bachelor of Applied Science in Analytical and Industrial Chemistry as well as Master in Chemical Instrumentation, Master and PhD by research. At the Physical Chemistry section, a total of 9 staff are involved in teaching of academic courses at the undergraduate and postgraduate levels. They are also actively conducting research in molecular modelling, green chemistry, environmental science, surface science and materials science such as zeolites, nanomaterials and layered materials.

2-OP 10:10

August 23 (Room207)

Chairman: Prof. Guan-Yeow Yeap

Synthesis, Characterization, Mesomorphic and Magnetic Properties of Trisubstituted Phenyl Derivatives Containing Biphenyl Ester and Aromatic Imine Fragments with *o*-Ethoxy Substituent

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Keywords: *Liquid crystal; calamitic; magnetic interaction; nematic phase*

ABSTRACT

A new series of calamitic trisubstituted phenyl derivatives obtained from the reaction of *p*-anisidine and 2-ethoxy-4-formylphenyl-4'-(octyloxy)-[1,1'-biphenyl]-4-carboxylate have been successfully isolated and characterized. This series consist of six homologous members with varying number of terminal alkoxy chains, C_nH_{2n+1} (n= 7-12). The molecular structures for all compounds have been elucidated by CHN elemental analysis, FT-IR, ¹H-NMR and ¹³C-NMR spectroscopic techniques. The thermal and mesomorphic behavior of the title compounds were observed using differential scanning calorimetry (DSC) and polarizing optical microscope (POM). As inferred from POM, all the target compounds exhibit enantiotropic nematic (N) phase. The observation also shows that the N phase temperature range for Schiff's base esters decreases when the length of the terminal alkoxy chains increases from n= 7 to n=12. Further investigation has shown that all the title compounds exhibit an unusual short-range magnetic interaction in which the compounds were attracted to the magnet in solid state as well as in the presence of water medium at elevated temperature.

3-OP 10:30

August 23 (Room207)

Chairman: Prof. Guan-Yeow Yeap

Synthesis, Characterization and Biological Studies on Fluorene-based compounds armed by pyridine and quinoline

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Key words: Fluorene-based heterocyclic compound; nuclear magnetic resonance; infrared; in-vitro cytotoxicity; antimicrobial; DPPH scavenging activity

ABSTRACT

New heterocyclic compounds containing pyridine and quinoline connected to fluorene core, 1,1'-(9,9-dihexyl-9H-fluorene-2,7-diyl)bis(N,N-bis(pyridine-2-ylmethyl)methanamine (**1**) and 8,8'-(((9,9-dihexyl-9H-fluorene-2,7-diyl)bis(methylene))bis(oxy))diquinoline (**2**) have been successfully synthesized in exceptionally good yield of 60% and 63%, respectively. The molecular structure of the synthesized compounds was well characterized by nuclear magnetic resonance (NMR), infrared (FTIR), and UV-vis absorption techniques. The biological activities; *in-vitro* cytotoxicity, antimicrobial and antioxidant activities of the synthesized compounds were investigated. The *in-vitro* cytotoxicity activity of the compounds (**1**) and (**2**) was evaluated against human cervical (HeLa) cancer cell line. Target compounds demonstrated antimicrobial activity through disc diffusion assay performed on *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, *Candida albicans* and *Saccharomyces cerevisiae*. Antioxidant activity of the target compounds were demonstrated by DPPH radical scavenging activity.

4-OP 11:00

August 23 (Room207)

Chairman: Prof. Shinsaku Maruta

Photo-regulation of Small GTPase Ras using photochromic molecules

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Key words: Small GTPase, Ras, Photochromic, Peptide inhibitor, Protein domain mimetics

ABSTRACT

Small GTPase Ras is known as a central regulator of cellular signaling. Ras has well studied at molecular level because its mutation cause tumor formation. Also it is already known that Ras serves as molecular switch and it was regulated by two kinds of factors, GEFs(SOS) and GAPs. Nowadays, some researchers focused on Ras-SOS interaction and reported mimic peptide of SOS's alpha-H helix region inhibitor actually inhibited Ras activity competitively with SOS. However, these reported mimic peptides were unstable in solution without specific modification because of its short length. Before, our lab succeeded to synthesize azobenzene derivatives, ABDM which have two cysteine reactive moiety at both ends, and it can change its structure dynamically by UV and VIS light irradiation reversibly accompanied with Cis/Trans isomerization. Here we designed SOS mimicking peptide which have two cysteines at cross-linkable position in order to modify it with ABDM. We examined that ABDM modification of designed peptide actually stabilized peptide secondary structure. Also, our peptide at Trans form of ABDM strongly inhibited Ras activity than Cis forms and this indicated that isomerization of ABDM broke peptide secondary structure from the result of CD spectrum.

5-OP 11:20 August 23 (Room207) Chairman: Prof. Shinsaku Maruta

Photochromic inhibitor composed of spiropyran or azobenzene can photoregulate the kinesin Eg5 activity.

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Key words: Kinesin Eg5, inhibitor, photochromism, spiropyran, azobenzene

ABSTRACT

The mitotic kinesin Eg5, a member of the kinesin-5 family, is a plus-end directed homotetrameric molecular motor. Eg5 is essential for the formation of bipolar spindles and is considered for a target of anti-cancer drug. Previously many inhibitors of Eg5 have been developed as anticancer drugs. Interestingly, although the inhibitors have no conserved structure, they bind to the common pocket composed of L5, $\alpha 2$ and $\alpha 3$ in Eg5 motor domain. In this study, we synthesized novel photochromic Eg5 inhibitors, DSPPA and BDPSB composed of two spiropyran derivatives or two azobenzene derivatives, respectively. DSPPA exhibited hydrophobic spiro (SP) and polar merocyanine (MC) isomerization upon visible and UV light irradiations, respectively. SP-DSPPA inhibited more significantly ATPase and motor activities than MC isomer. BDPSB exhibited trans and cis isomerization upon visible and UV light irradiations, respectively. Trans-BDPSB significantly inhibited Eg5 ATPase activity and motor activity than cis-BDPSB. The results suggest that the photochromic inhibitors exhibits highly efficient for photo-switch.

6-OP 11:40 August 23 (Room207) Chairman: Prof. Shinsaku Maruta

Photo-regulation of mitotic kinesin Eg5 using photochromic compounds which forms three isomerization states

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Key words: Kinesin Eg5, inhibitor, photochromism, spiropyran, azobenzene

ABSTRACT

Eg5 is a ATP drive motor protein, which moves along microtubules to carry various kinds of cargoes. It controls chromosomal segregation in mitosis and is thus a critical drug target for cancer therapy. There is some antimitotic drugs such as Taxanes bind to the tubulin and block the cell cycle progression at mitosis through the interruption of microtubule dynamics which ultimately result of cell death. In addition, anti-microtubule agents also caused peripheral neuropathy as an adverse event by interfering with microtubule-based axon transport. Therefore, antimitotic agents that target the components of mitotic machinery other than microtubule has been considered as a potential target for cancer treatment. Several specific and potent inhibitors of Eg5 are known as such Monastrol, STLC, Ispinesib etc. But the structure of those inhibitor is not conserved and show diversity. In my study, to control mitotic kinesin Eg5, I have synthesized a novel photochromic compound composed of azobenzene and Spiropyran and 2,3-dimercaptosuccinic acid derivatives. The photochromic compound SP-AB formed Merocyanine-Cis, Spiro-Trans and Merocyanine-Trans states depend upon ultraviolet irradiation, Visible Light irradiations, and in the dark respectively. The ATPase activity of Eg5 is inhibited by the inhibitor in the presence or absence of microtubule as a photo-switch respectively.

7-OP 14:00

August 23 (Room207)

Chairman: Prof. Akio Shimizu

The influence of molecular structure of ionic liquids on cellulose solubility

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Key words: Ionic liquids, Cellulose, Solubility, Polarity parameter

ABSTRACT

Cellulose solubility of ionic liquids (ILs): 1-alkyl-3-methylimidazolium acetate ($[C_n\text{MIm}][\text{Ac}]$) with different alkyl chain length ($n=0, 2, 4$) and dimethyl sulfoxide (DMSO) mixture was investigated in an attempt to obtain a deep insight into cellulose solvation behavior. Cellulose solubility was examined with IL mole fraction of 0~0.25 in which IL concentration does not cause viscosity interference of cellulose dissolution. As IL concentration increases, cellulose solubility increases almost linearly up to 0.25 IL mole fraction of DMSO mixture. In spite of different cation combination, $[C_2\text{MIm}][\text{Ac}]$ and $[C_4\text{MIm}][\text{Ac}]$ had similar cellulose solubility at each IL concentration, indicating that difference in alkyl chain length of C_2 and C_4 have little effects on cellulose dissolution capacity. However, even pure $[C_0\text{MIm}][\text{Ac}]$ could not dissolve cellulose at all. This result was closely related with polarity parameter called β value (hydrogen bond basicity). Although β value of $[C_2\text{MIm}][\text{Ac}]$ and $[C_4\text{MIm}][\text{Ac}]$ showed 1.109 and 1.201, respectively, $[C_0\text{MIm}][\text{Ac}]$ had 0.680. Since 0.8 of β value is required for cellulose dissolution, the non-dissolving capacity of cellulose can be explained. We would like to introduce the additional findings on more variety of ILs with different alkyl chain length as well on the day of our presentation.

8-OP 14:020

August 23 (Room207)

Chairman: Prof. Akio Shimizu

Temperature dependence of solution structure from dynamic properties of Propylammonium nitrate/water mixtures.

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Key words: Protic Ionic Liquid; Self-diffusion coefficient; Viscosity; nano-domain structure; α value

ABSTRACT

Ionic liquids (ILs) are salts with melting points below 100 °C. ILs have many unique characteristics, including negligible vapor pressures, refractory properties and high thermal stability. Unlike molecular liquids, which are homogeneous, ILs contain both polar and nonpolar regions, and thus tend to undergo flocculation to form a special nano-domain structure that is inhomogeneous on the nanoscale. This structure has been examined from a static perspective using molecular dynamics simulations in a number of ILs, including 1-butyl-3-methylimidazolium tetrafluoroborate. Also, it is suggested that water puddles which was called as "water pocket" exist in IL/water mixture. Therefore, the physicochemical properties of IL/water mixture have attracted many researchers interest. In addition, in the amine-based IL, those having an intermediate phase called soft viscous crystals have been discovered instead of liquid crystals. However, the physicochemical properties of such solutions are not fully investigated. In this study, we report the physicochemical properties of propylammonium nitrate/ water mixtures from a dynamic point of view. As a comparison, Propylamine which is a molecular solvent was also investigated. Specifically, we determined α values, which indicates solution homogeneity, from solution viscosity and self-diffusion coefficient of each component in solution at various temperature.

9-OP 14:40

August 23 (Room207)

Chairman: Prof. Akio Shimizu

Mitigation of Toxic *Alexandrium Tamiyavanichii* using Chitosan-silica Composite

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Key words: Toxic algae; silica; chitosan; rice husk ash; rice husk; Alexandrium Tamiyavanichii

ABSTRACT

The harmful algal blooms (HABs) phenomena affect human health, fishing and tourism industries. In a single occasion, the loss due to HABs can reach thousands of Ringgit Malaysia. In this study, chitosan-silica composite (RHA-CHI) was synthesized via sol-gel technique for the mitigation of *Alexandrium tamiyavanichii*, a toxic HAB species isolated from Malaysian waters. Rice husk ash silica was used as the silica precursor in the composite synthesis. The FT-IR spectroscopy suggests that chitosan was covalently bonded with the surface silanol groups. Light microscope analysis indicates that the algal cells stick on the surface of the composite and underwent lysis. The removal efficiency of *A. tamiyavanichii* was 75 % using 0.1 mg/ml of RHA-Chi in 2 hours, increasing to 85% after 24 hours whereas the removal efficient was 16% using only silica. The findings show that chitosan-silica composite has high potential to be used in mitigation of HAB species, particularly *A. tamiyavanichii*.

Coffee Break (15:00-15:10)

10-OP 15:10

August 23 (Room207)

Chairman: Prof. Afidah Abdul Rahim

Photosensitive Polymers Containing Benzylidene Ketone as Florescent Chemosensor for Heavy Metal Ions

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Key words: Photosensitive polymer; benzylidne ketone; fluorescence; photocrosslinking; chemosensors

ABSTRACT

Photosensitive polymers bearing the benzylidene ketone in the back bone or in the side chain were synthesized. The benzylidene ketone moiety was introduced in the polymers because of its versatile photo-active property and special features like high thermal stability, photo-curing ability, electronic conductivity and fluorescence. The photoreactivity of benzylidene mono ketone based polymers revealed that the olefinic double bonds of the benzylidene ketone groups dimerized and led to photocrosslinking. The luminescence intensities of the crosslinked polymers were enhanced, illustrating that effective π - π stacking interaction among the phenyl rings may occur due to aggregation of the polymeric chains. This suggested that the polymers possessed an aggregation-induced emission enhancement characteristic. The potential of the polymers as chemosensor was investigated using various heavy metal ions. The synthesized polymers containing benzylidene mono ketone showed 'turn on' fluorescence behavior as heavy metal ions were titrated into each of the polymer solutions. Whereas, curcumin based polymer which contains benzylidene β -diketone acted as 'turn off' fluorescent chemosensor. Some of the synthesized polymers illustrated sensitivity and selectivity towards specific metal ions as well.

11-OP 15:30 August 23 (Room207)

Chairman: Prof. Afidah Abdul Rahim

Artificial tactile nerves based on hetero-core optic fiber sensors

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Key words: Tactile sensing, fiber optic sensor, hetero-core

ABSTRACT

This paper reports a novel technical approach for mimicking human sense of touch based on hetero-core fiber optic sensors. Human skin serves as one of essential interfaces to understand environments, objects and other humans, so that the tactile sense of human also provides a variety of information such as a shape, position and physical nature of objects, comfortability of products, and furthermore emotion of other human. Hetero-core fiber optic sensors consist of two optical fibers fusion-spliced with different core diameters so as to obtain light leakage depending on bending curves in sensory portion. It also performs as artificial sensory nerves detecting the deformation of soft materials with comfortability and high robustness against environmental changes. The hetero-core fiber sensor was proved to detect both static and dynamic contact forces in such a way to embed into a pseudo-finger device made of soft silicone elastomer. It has also been demonstrated that the response of the sensor inside a pseudo-finger was in good agreement with a stress relaxation curves, and therefore had a ability to discriminate touched objects with respect to physical nature.

12-OP 15:50 August 23 (Room207)

Chairman: Prof. Afidah Abdul Rahim

Trace measurement with optical fiber spectroscopic cell fabricated by femtosecond laser

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Key words: Femtosecond laser drilling, Optical fiber sensor, Localized surface plasmon resonance, Gold nanoparticles, Biological sensing

ABSTRACT

A novel spectroscopic measurement method has been established that enables to detect biomolecules in a simple measurement configuration with a small absolute amount of sensing targets. A microhole penetrating a glass optical fiber was fabricated by femtosecond laser drilling. The microhole works as an optical fiber spectroscopic cell which has sensing volume of sub-picoliters, since the spectroscopic cell is capable of interacting liquid samples introduced into the cell with propagating light in the optical fiber. By use of the cell with a combination of a halogen white light source and a compact CCD spectrometer, spectroscopic measurements using localized surface plasmon resonance (LSPR) were demonstrated. Absorption spectra using LSPR, which had the absorption peak centered at 518 nm, were obtained when a solution of gold nanoparticles (GNPs) with a diameter of 5-10 nm was injected into the cell with a volume of 0.4 pL. An aggregation of GNPs caused by biomolecules of L-cysteine was monitored by the change in the absorption spectra. The absorption peak of LSPR decreased due to an injection of 7.5 mM of L-cysteine with the detection sensitivity of 3.0×10^{-15} mol (3.6×10^{-13} g).

Coffee Break (16:10-16:20)

13-OP 9:30

August 24 (Room207)

Chairman: Prof. Junichi Ida

Removal of Heavy Metals using S-Quinolin-2-yl-Methyldithiocarbazate Functionalized Magnetic Nanoparticles

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Key words: Magnetic nanoparticles; S-quinolin-2-yl-methyldithiocarbazate; heavy metals removal

ABSTRACT

S-quinolin-2-yl-methyldithiocarbazate based magnetic nanoparticles (MNP-SQ2MDTC) as heavy metal adsorbent was synthesized and assessed its adsorption capabilities. MNP-SQ2MDTC adsorbent was prepared by refluxing MNPs (Fe₃O₄) with SQ2MDTC and sodium bicarbonate in dry toluene with constant stirring. The surface of MNPs was first coated with 3-aminopropyltriethoxysilane (APTES) as cross-linker and then SQ2MDTC was covalently incorporated to the coated MNPs. The structural and surface characteristics of the obtained nanoparticles were investigated by FTIR, CHNS elemental analysis, TGA, XRD, FESEM and BET analysis. The SQ2MDTC functionalized MNPs exhibited high adsorption affinity for aqueous Cu(II) and Pb(II) ions when analysed using ICP-OES, resulting from complexation of the metal ions by surface amino groups. Findings of the present work highlighted the potential of MNP-SQ2MDTC as an effective adsorbent for the removal of heavy metal ions in water and wastewater treatment.

14-OP 9:50

August 24 (Room207)

Chairman: Prof. Junichi Ida

Alkali Metal Hydrides Modification on Chemical Hydrides for Improved Dehydrogenation

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Key words: Hydrogen storage; dehydrogenation; chemical hydrides; alkali metal hydrides

ABSTRACT

One of the main reasons for the sluggish progression in the realization of hydrogen economy lies in the challenge to store hydrogen efficiently. The US DOE has set rather challenging hydrogen storage target, such as system gravimetric capacity of 4.5 wt% and system volumetric capacity of 3.0 kg H₂/L by 2020. In order to solve the hydrogen storage problem, flurry of research has been devoted to explore new materials with high hydrogen capacity. However, none of the materials meet the entire set target. Materials of our interest include chemical hydrides largely due to their attractive hydrogen storage capacities. Chemical hydrides such as ammonia borane and hydrazine borane possess exceptionally high hydrogen content of 19.6 wt% and 15.4 wt%. However, they suffer from slow dehydrogenation kinetics, unfavorable dehydrogenation thermodynamics, foaming and emission of unfavorable by-products. In our research, we have been working on chemical modification on these chemical hydrides using various metal hydrides and discovered several fascinating structures, which also exhibit greatly enhanced hydrogen storage properties. For example, bimetallic sodium magnesium amidoborane exhibited an endothermic dehydrogenation at moderate temperatures with much improved hydrogen purity and no significant foaming issue. Similarly, metal hydrazidoboranes demonstrated enhanced dehydrogenation kinetics with greatly suppressed by-product formation.

15-OP 10:10

August 24 (Room207)

Chairman: Prof. Junichi Ida

A Simple Synthesis Method of Thermoresponsive Polymer Immobilized Magnetite Nanoparticles for Heavy Metal Ions Recovery

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Key words: Adsorption, Magnetite nanoparticles (MNP), Thermoresponsive polymer

ABSTRACT

We have been developed straight chained thermoresponsive heavy metal ions adsorbent incorporating N-isopropylacrylamide (NIPAM) and Acrylic acid (AA). In this study, to enhance the reusability of the adsorbent, we tried to immobilize it onto magnetite nanoparticle (MNP). The conventional polymer immobilization methods onto nanoparticle have a disadvantage that the processes are complicated, and take long time. The purpose of this study is 1) to simplify the immobilization process during the synthesis of our adsorbent and 2) to evaluate the heavy metal ions recovery ability of the adsorbent.

In the experiment, immobilization of poly(NIPAM-co-AA) onto MNP was carried out by applying Tural et al. coprecipitation method. First, poly(NIPAM-co-AA) was mixed in iron ion solution beforehand. Then, alkaline solution was dropped to obtain sample. The experimental results showed that poly(NIPAM-co-AA) was successfully immobilized on MNP. The results of the Cu (II) adsorption experiment showed that the recyclable amount of Cu (II) was 0.13 mmol/(g-adsorbent) at the maximum when temperature swing was carried out between 60°C and 20°C. Despite the simple method, the adsorbent showed the almost the same value as other thermoresponsive adsorbents which were prepared by the complicated conventional methods. These results indicated that the reusable thermosensitive adsorbent with high heavy metal recycling ability can be synthesized by our comparatively simple method.

Coffee Break (10:30-10:50)

16-OP 10:50

August 24 (Room207)

Chairman: Prof. Masato Ito

Preparation of Amine Modified Bimodal Mesoporous Silica Particles for CO₂ separation

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Key words: CO₂ adsorption, Bimodal mesoporous silica, Polymethylhydrosiloxane

ABSTRACT

Mesoporous silica has been extensively studied for many applications such as CO₂ adsorbents, drug delivery, catalysis, and so on. Among them, bimodal mesoporous silica (BMS), which had two different sizes of mesopores, have drawn much attention recently because it exhibited unique diffusion properties in the pores. For this reason, when BMS is modified to have affinity with CO₂, it is expected that high CO₂ adsorption capacity is obtained by small pores and fast adsorption rate is achieved by large pores. Therefore, we prepared various kinds of amine modified BMS, and the effects of pore structure of BMS samples and the type of introduced amine on CO₂ adsorption/desorption properties were examined in this study. In the experiments, various BMS samples were prepared with different Polymethylhydrosiloxane (PMHS) concentration as template for large pores, and the pore structures of the resulting samples were investigated. As a result, preparation procedure of bimodal mesoporous silica (BMS) with different pore structure was established in this study. Then, the effect of pore structure on CO₂ adsorption characteristics was examined using the resulting BMS samples after modifying with various amino groups. The results showed that by applying BMS for CO₂ adsorption, it was found that high CO₂ adsorption capacity was achieved by small pores and fast adsorption rate was achieved by large pores as expected.

17-OP 11:10

August 24 (Room207)

Chairman: Prof. Masato Ito

Effect of power frequency on various organic compounds(VOCs) decomposition using nonthermal plasma reactor combined with ceramic filter

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Key words: VOCs, Non-thermal plasma, TCE, Benzene

ABSTRACT

Recently, volatile Organic Compounds(VOCs) emissions have been controlled in various countries in the world. Nonthermal plasma decomposition method has been drawing more attention these days as an alternative approach for VOCs decomposition because of its advantages over conventional methods. In our previous work, we developed a new type electrode system for gas treatment in which nonthermal plasma and a ceramic filter were integrated and applied it for VOCs treatment.

In this study, in order to investigate the effect of both power frequency and chemical structure of VOC on the decomposition efficiency, discharge decomposition experiment of various VOCs was carried out using our plasma reactor. In the experiment, trichloroethylene (TCE), n-hexane, benzene, n-pentane, 1-hexene, 1-chlorohexane were used as VOCs to be decomposed, and the power supply frequencies were changed to perform discharge decomposition. As a result, in the case of 1-hexene and TCE, very high decomposition efficiency was shown, and at the same time, the decomposition efficiency was significantly influenced by the power frequency. On the other hand, the decompositions of 1-chlorohexane, n-hexane, n-pentane and benzene were influenced by the power frequency slightly, and the decomposition efficiency was remarkably lower than the case of 1-hexene and TCE.

18-OP 11:30

August 24 (Room207)

Chairman: Prof. Masato Ito

Software for handling the WURCS glycan representation

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ABSTRACT

WURCS is a universal glycan strong representation we have developed to be able to uniquely represent any glycan, otherwise known as a carbohydrate sugar chain. We have been developing software for drawing and representing various types of glycans. First, we have extended GlycanBuilder to be able to draw cyclic glycans, fragmented glycans and repeated glycan structures. The drawn glycans can also be exported as figures or as various text formats. Moreover, an importer has been incorporated into GlycanBuilder to be able to take WURCS as input to draw on the canvas. We have also developed the GlycanFormatConverter software so that existing text representations of glycans such as IUPAC and KCF can be translated into WURCS. To validate this converter, we tested the conversion to and from these other formats to see if the WURCS text before and after conversion matched. We were able to glean various insights during this validation procedure while showing that our tool could accurately convert between these formats.