

# Synthesis of Functional Phenolic Resins and Analysis of Their Formation Reaction by Computer

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# 1988 Fiscal Year Final Research Report Summary

## Synthesis of Functional Phenolic Resins and Analysis of Their Formation Reaction by Computer

Research Project

### Project/Area Number

62550668

### Research Category

Grant-in-Aid for General Scientific Research (C)

### Allocation Type

Single-year Grants

### Research Field

高分子合成

### Research Institution

KANAZAWA UNIVERSITY

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### Project Period (FY)

1987 - 1988

### Keywords

PHENOLIC RESIN / CALIXARENE / HOST-GUEST INTERACTION / COMPUTER SIMULATION / TEMPERATURE / MOLECULAR CONFORMATION / HYDROGEN BONDING / 分岐

### Research Abstract

The synthesis, the reaction mechanisms and the solution properties of the phenolic resins were studied and the following results were obtained.

1. The synthetic method of calixarene, the cyclic phenolic oligomer, in high yield and in high selectivity were established. By the esterification and the etherification and by the bonding into acrylic resin and epoxy resin, calixarene became widely applicable. The host-guest interaction of calixarene for organic molecules and the structure of their clathrate complexes were discussed.
2. The formation reaction of the phenolic resin in early stage is so complex that some elemental reactions had to be considered. Since it is impossible to

obtain the rate of each elemental reaction by usual organic technique, our computer simulation method was successfully applied.

3. The phenolic resins whose molecular structures were definite were prepared to discuss the molecular conformation in solution. At first, temperatures for some phenolic resin-solvent systems were determined from phase equilibrium measurements, and then the molecular conformation in a good solvent and in a solvent were discussed. It was known that the molecules of the phenolic resins shrink considerably because of the contribution of the intramolecular hydrogen bonding between phenolic hydroxyl groups and the branching, and therefore, acetylated o-cresol resin which has not any phenolic hydroxyl groups and any branches behave as an unperturbed chain in condition.

## Research Products (11 results)

All Other

All Publications (11 results)

- [Publications] KOMOTO,TADASHI: Journal of the Chemical Society,Chemical Communications. 1988. 135-136 (1988) ▼
- [Publications] 中本義章: 金沢大学工学部紀要. 21. 119-124 (1988) ▼
- [Publications] SUE,HARUAKI: Journal of Applied Polymer Science. ▼
- [Publications] SUE,HARUAKI: Polymer Bulletin. 21. 97-104 (1989) ▼
- [Publications] 中本義章: 熱硬化性樹脂. 10. (1989) ▼
- [Publications] 中本義章: 熱硬化性樹脂. 10. (1989) ▼
- [Publications] Tadashi Komoto: "A <sup>13</sup>C Cross Polarization-Magic Angle Spinning N.m.r. Study of the Structure of p-t-Butylcalix[4]arene-Toluene Clathrate in the Crystalline State" Journal of the Chemical Society, Chemical Communications. 1988. 135-136 (1988) ▼
- [Publications] Haruaki Sue: "Determination of Mark-Houwink-Sakurada Equation for Phenolic Resins and Estimation of their Conformation in Acetone Solution" Journal of Applied Polymer Science. ▼
- [Publications] Haruaki Sue: "Determination of Mark-Houwink-Sakurada Equation for Phenolic Resins Containing Alkylenediamine in the Main Chain and Estimation of Their Molecular Conformation in Tetrahydrofuran" Polymer Bulletin. 21. 97-104 (1989) ▼
- [Publications] Yoshiaki Nakamoto: " Temperature and Molecular Conformation of o-Cresol Resin" Netsukoukasei Jyushi. ▼
- [Publications] Yoshiaki Nakamoto: "Polycondensation of p-Phenylenediamine and Bis(hydroxymethyl)-p-cresol" Netsukoukasei Jyushi. ▼

URL: [https://kaken.nii.ac.jp/report/KAKENHI-PROJECT-62550668/625506681988kenkyu\\_seika\\_hokoku\\_](https://kaken.nii.ac.jp/report/KAKENHI-PROJECT-62550668/625506681988kenkyu_seika_hokoku_)

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