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Synthesis and structural characterisation of novel urethane-dimethacrylate monomers with two quaternary ammonium groups based on cycloaliphatic diisocyanates

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INTRODUCTION & AIM

High consumption of sugar may result in declining health—diseases such as obesity, diabetes or caries. Bacteria, existing in the human mouth, *metabolise* sugar into organic acids. These acids demineralize teeth causing caries. World Health Organization's report [1] from 2022 points out, that around 2 billion adult people and over 500 million children are affected by caries.

The caries is treated by the removal of infected tissue and filling the cavity with dental composite restorative material (DCRM). Such materials consist of inorganic filler (silica compounds) suspended in the polymeric matrix. DCRM modification is widely researched in literature [2-4], due to the neglect of antibacterial activity of commercial materials.

The aim this study was synthesis of two novel monomers possessing quaternary ammonium groups. The novel compounds were based on cycloaliphatic diisocyanates - isophorone diisocyanate (IPDI) and 4,4′-methylenebis(cyclohexyl isocyanate) (CHMDI).

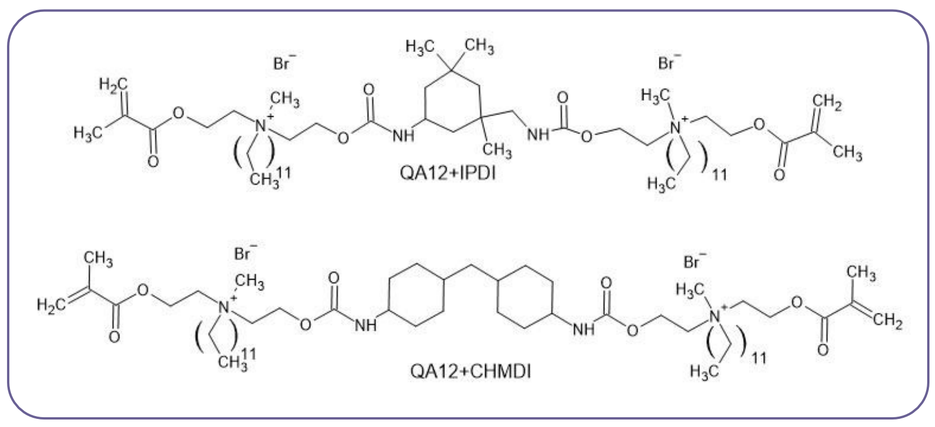

Fig.1. Chemical structures of QA12+IPDI and QA12+CHMDI.

METHOD

The three-step procedure was utilised to obtain the novel monomers:

1. Transesterification of methyl methacrylate (MMA) with N-methydiethanolamine (MDEA);

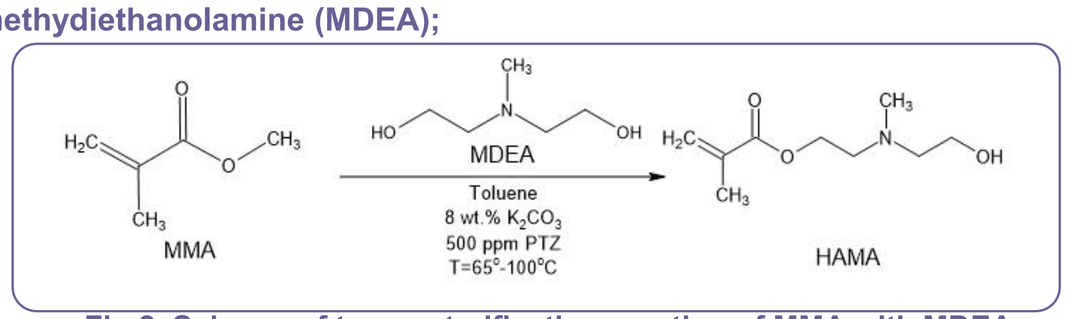

Fig.2. Scheme of transesterification reaction of MMA with MDEA.

2. N-alkylation of HAMA with 1-bromododecane;

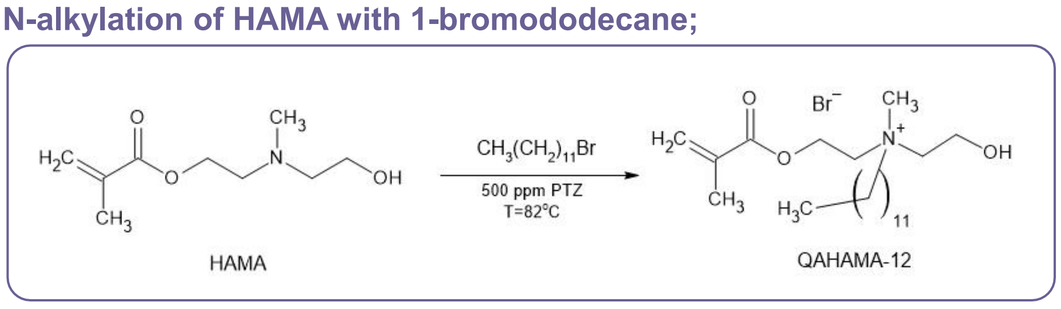

Fig.3. Scheme of N-alkylation reaction with 1-bromododecane.

3. Addition of QAHAMA-12 to diisocyanate.

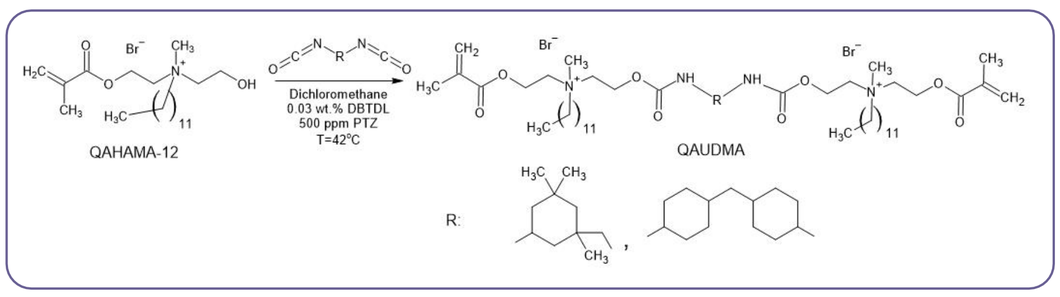

Fig.4. Scheme of addition to diisocyanate.

The structures of monomers were confirmed with 1H and 13C NMR and FTIR.

RESULTS & DISCUSSION

^{1}H NMR

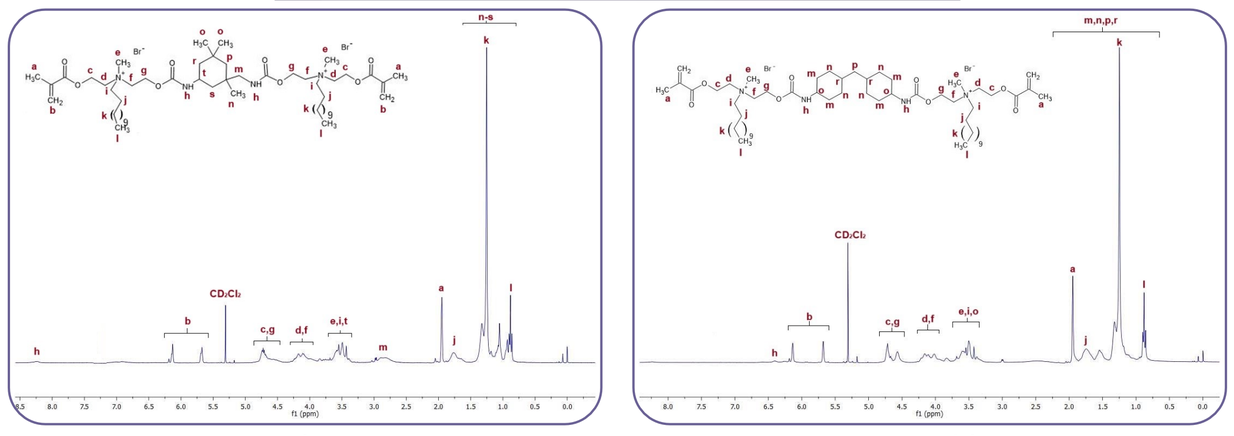

Fig.5. ^{1}H NMR Spectra of novel monomers: a) QA12+IPDI; b) QA12+CHMDI

^{13}C NMR

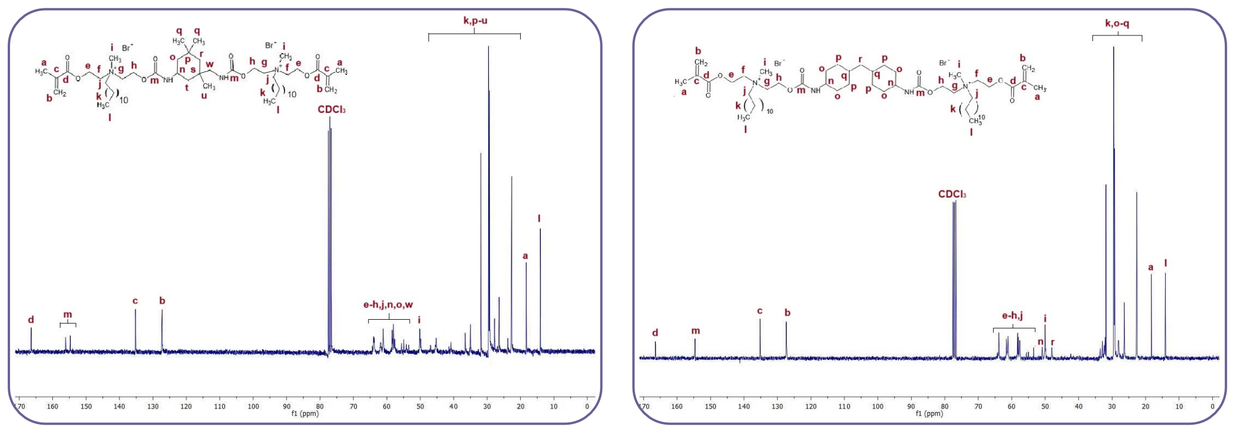

Fig.6. ^{13}C NMR Spectra of novel monomers: a) QA12+IPDI; b) QA12+CHMDI

FTIR

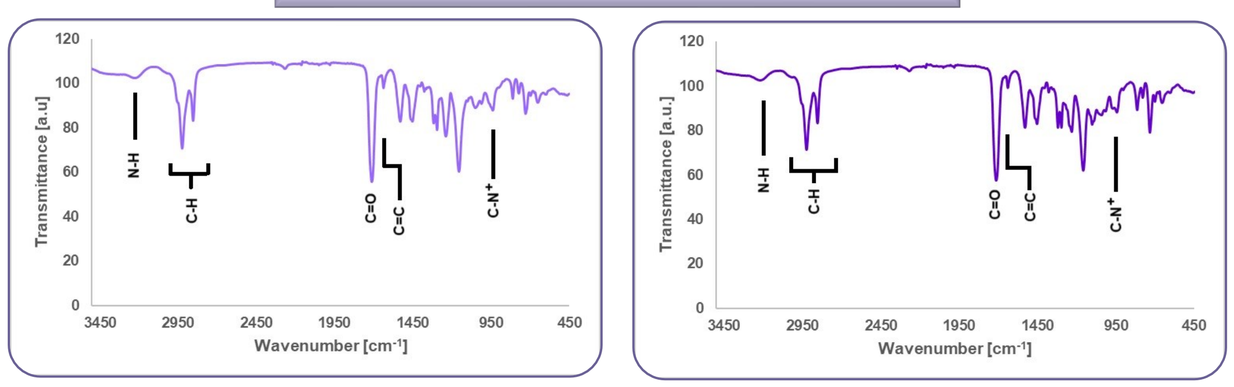

Fig.7. FTIR Spectra of novel monomers: a) QA12+IPDI; b) QA12+CHMDI

At ^{1}H and ^{13}C NMR spectra are visible peaks corresponding to key elements of the chemical structures of these monomers.

FTIR spectra confirmed the full conversion of diisocyanate to urethane bonds.

CONCLUSION

The novel monomers were successfully obtained. These monomers were yellowish, viscous resins. Their structures were confirmed with spectroscopy methods.

Future work should focus on determining the physicochemical properties of QA12+IPDI and QA12+CHMDI and their copolymers.

FUTURE WORK / REFERENCES

[1] WHO. Global Oral Health Status Report: Towards Universal Health Coverage for Oral Health by 2030; World Health Organization: Geneva, Switzerland, 2022.

[2] Zhang, Y.; Chen, Y.; Hu, Y.; Huang, F.; Xiao, Y. Quaternary ammonium compounds in dental restorative materials. Dent. Mater. J. 2018, 37, 183–191.

[3] Makvandi, P.; Jamaledin, R.; Jabbari, M.; Nikfarjam, N.; Borzacchiello, A. Antibacterial Quaternary Ammonium Compounds in Dental Materials: A Systematic Review. Dent. Mater. 2018, 34, 851–867.

[4] Featherstone, J. Dental restorative materials containing quaternary ammonium compounds have sustained antibacterial action. J. Am. Dent. Assoc. 2022, 153, 1114–1120.