Efficient Synthesis of Nitrile Compounds via Direct Substitution of Aliphatic Polycarboxylic Compounds.

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Abstract

This study introduces an innovative method for synthesizing aliphatic nitrile compounds through a direct substitution reaction between aliphatic compounds containing two or more carboxyl groups and nitrile compounds. The novel approach offers an efficient pathway to convert multi-carboxylic functional groups into nitrile functionalities, enabling the production of a wide range of aliphatic nitrile compounds with enhanced structural and functional versatility.

The process leverages direct substitution reactions under optimized conditions, minimizing the need for intermediate steps and excessive reagents. Key experimental parameters, such as catalyst selection, reaction temperature, and time, were systematically optimized to achieve high yield and selectivity. The resulting nitrile compounds have potential applications in various industrial fields, including pharmaceuticals, polymers, and specialty chemicals.

This innovative approach not only improves the efficiency of nitrile synthesis but also aligns with sustainable chemical practices by reducing byproduct formation and energy consumption. The method is expected to contribute significantly to the advancement of aliphatic nitrile compound production, providing new opportunities for industrial applications and academic research.

Keywords : Aliphatic nitrile compounds, direct substitution, multi-carboxyl groups, sustainable synthesis, industrial applications

Background

- **Aliphatic nitrile compounds**—in particular, adiponitrile (ADN)—are indispensable intermediates in nylon-6,6 production.
- ADN is hydrogenated to hexamethylenediamine (HMDA), which then reacts with adipic acid to yield the high-performance polyamide nylon-6,6.
- Nylon-6,6 finds broad application in the **automotive**, **electronics** and **textile** sectors.
- Over **90%** of global ADN output is funneled into nylon-6,6 manufacturing.
- Conventional ADN syntheses remain **energy-intensive** and **environmentally taxing**, driving the pursuit of **more sustainable**, **efficient routes**.

Objective

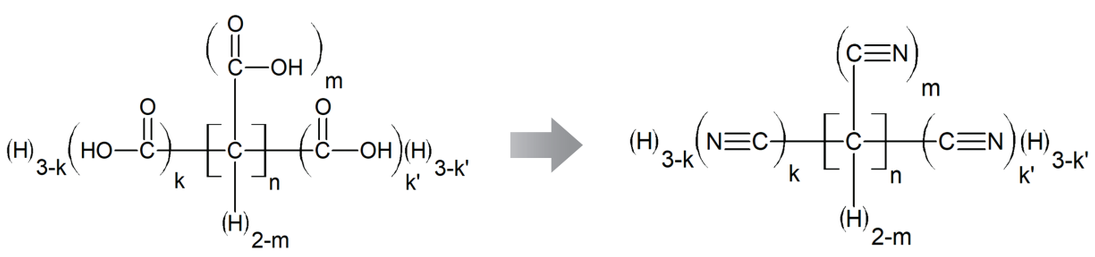
Develop a green and efficient method to synthesize aliphatic nitrile compounds :

- No catalyst
- High product purity
- No water washing step
- Recyclable reactants

[Comparison of Aliphatic Nitrile Compound Synthesis Methods]

	Feedstock	New Method According to Invention
Feedstock	Olefin (unsaturated hydrocarbon)	Aliphatic compound with two or more carboxyl groups
Reaction Approach	Chiorination followed by cyanide substitution or hydrocyanation	Direct substitution reaction (carboxyl group → nitrile group
Catalyst/Additive Use	Nickel catalyst, acid chlorinating agents, etc, required	No catalyst, no additives
Reaction Conditions	High temperature, high pressure, organic solvent present	Few impurities. high-purity product obtainable
Product Purity	Numerous impurities, requires purification	Simple separation sufficient, no wahing process required
Purification Process	Multi-step washing and separation required	Minimal wastewater generation. environmentally friendly process
Environmental Impact	Difficult to reuse feedstock or solvent	Nitrile compound can be reused
Example Reactants	Olefin, hydrogen cyanide, nickel catalyst	Adipic acid, suberic acid, azelaic acid etc, + hydrogen cyanide, acetonitrile, butyronitrile, etc

Reaction Scheme



In the above chemical formula, **n** is an integer of 2 or greater, **m** is an integer ranging from 0 to 2 for each of the **n** carbon chains, and **k** and **k'** are integers ranging from 0 to 3, respectively.

Experimental Procedure

1. Mix dicarboxylic acid (e.g., adipic, sebacic, suberic acids) with acetonitrile.
2. React under supercritical conditions (260–500 °C, 40–200 bar) for 4 hours.
3. Separate products by depressurization and distillation.
4. Recycle unused reactants.

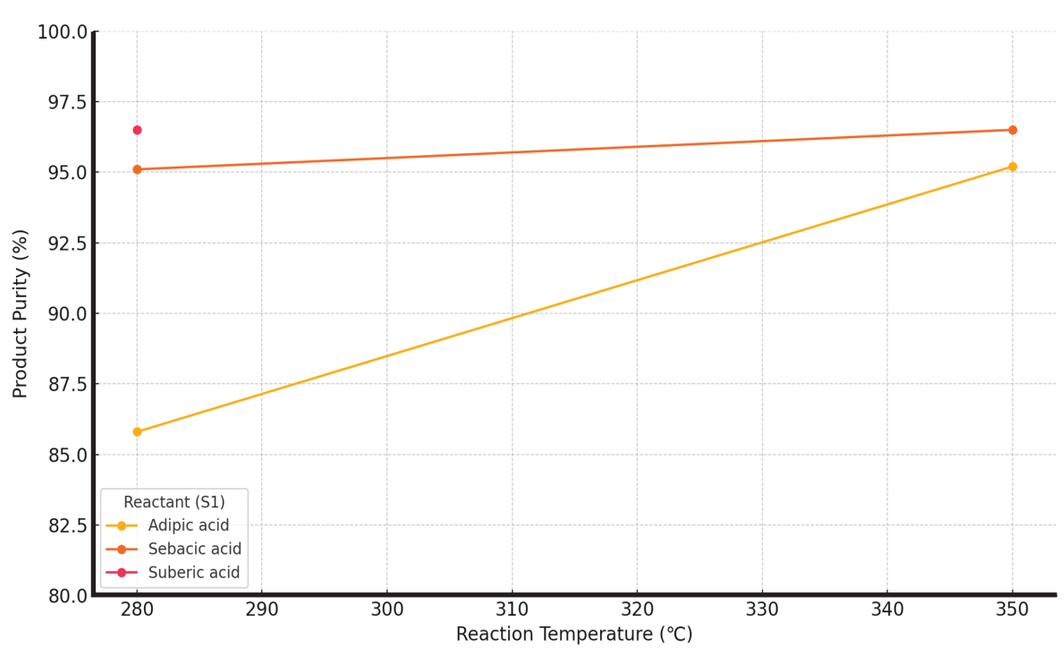
Results & Discussion

- Long-chain dicarboxylic acids yielded over 96% purity (seb., sub.)
- Short-chain acids (e.g., maleic, succinic) failed to form desired nitrile products.
- Water content in products was below 50 ppm.
- GC analysis confirmed product quality.

[Table 1. Synthesis Results of Aliphatic Nitrile Compounds]

Entry	S1 (Aliphatic acid)	S2 (Nitrile)	Temp. (℃)	Pressure (bar)	Time (hr)	Moisture (ppm)	Purity (%)
Example 1	Adipic acid	Acetonitrile	280	90	4	26	85.8
Example 2	Adipic acid	Acetonitrile	350	90	4	25	95.2
Example 3	Sebacic acid	Acetonitrile	280	90	4	29	95.1
Example 4	Sebacic acid	Acetonitrile	350	90	4	31	96.5
Example 5	Suberic acid	Acetonitrile	280	90	4	28	96.5
Control 1	Maleic acid	Acetonitrile	280	90	4	-	-
Control 2	Succinic acid	Acetonitrile	280	90	4	-	-
Control 3	Glutaric acid	Acetonitrile	280	90	4	-	-

[Effect of Reaction Temperature on Product Purity]



Conclusion

- High-yield, high-purity nitrile synthesis achieved without catalysts
- Environmentally friendly and economically viable
- Suitable for scale-up and electrolyte additive production

Inquiries and Contact Information

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