

New Substances Program Advisory Note 2006-01

New Substances Notification Technical Guidance Document: Reaction Scheme

The New Substances Notification (NSN) Technical Guidance Series was developed to help interpret specific information requirements of the *New Substances Notification Regulations (Chemicals and Polymers)* (the Regulations) of the *Canadian Environmental Protection Act, 1999* (the Act).

This document addresses the reaction-scheme requirement prescribed in Schedule 9 of the Regulations for polymers that meet the Reduced Regulatory Requirement criteria. It also provides background information and suggested formats for reporting polymer reaction schemes.

Background

A polymer-reaction scheme describes the step-by-step synthesis of a polymer and includes its intermediates, pre-polymers, and reaction by-products. Reaction-scheme information was not a regulatory requirement within the *New Substances Notification Regulations* published in July 1994. However, because this information is now recognized as valuable for evaluation, it has been added as a requirement. Knowledge of a polymer's reaction scheme enables government evaluators to determine structural variances of the polymeric product, potential by-products, and the presence or absence of various functional groups.

Scientific Rationale

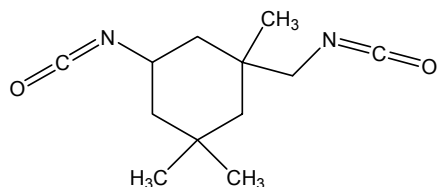
Because monomers are multifunctional, it can be difficult to establish the final polymer structure without an understanding of the reaction sequence. The provision of detailed reaction-scheme information will help confirm the Reduced Regulatory Requirement (RRR) status of the polymer and contribute to more accurate evaluations. The reaction scheme should contain the following information:

- The chemical identity of monomers, pre-polymers, and reactants in the polymer;
- The details of polymer synthesis, including the sequence of the addition of the monomers and reactants and their percent by weight and the relative number of moles;
- The nature of the reactions (for example, hydrolysis, epoxidation, or esterification); and
- The polymer structure and any known by-products.

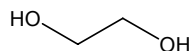
The reaction scheme is not intended to be a process description. In other words, it does not need to include an engineering diagram outlining such details as reaction vessels and storage and transport containers.

These two examples illustrate how the regulatory status of a polymer can be affected by changes in the order of the monomers and their molar ratios. The same three monomers are for the synthesis of both polymers:

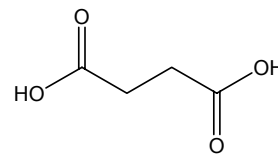
A) Isophorone diisocyanate



B) Ethylene glycol

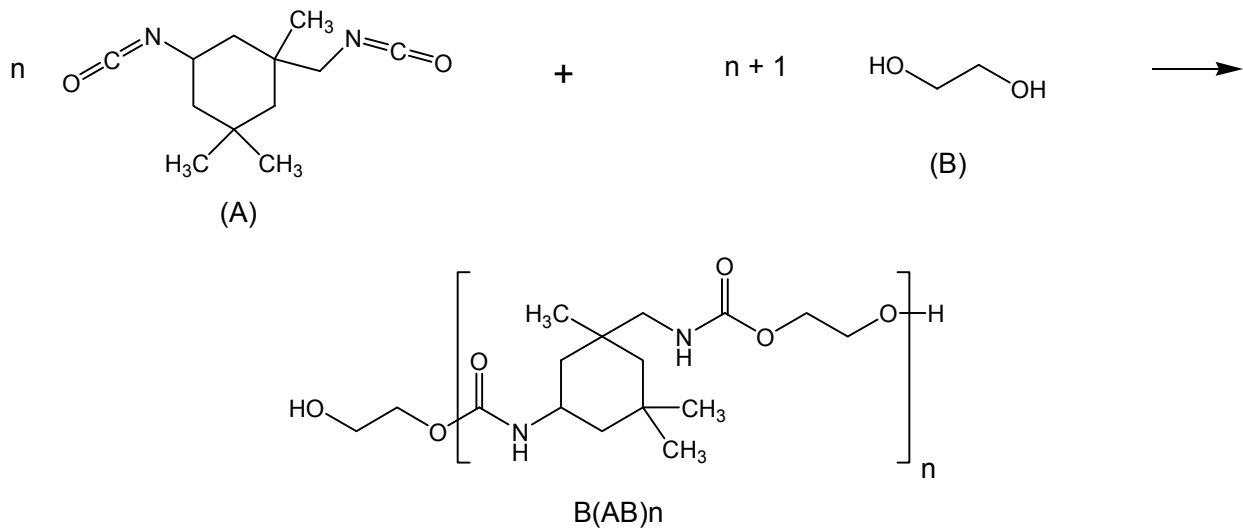


C) 1,4-butanedioic acid

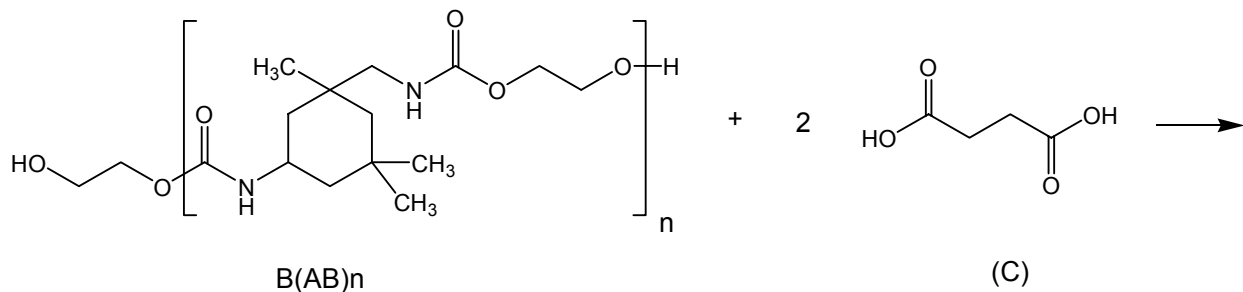


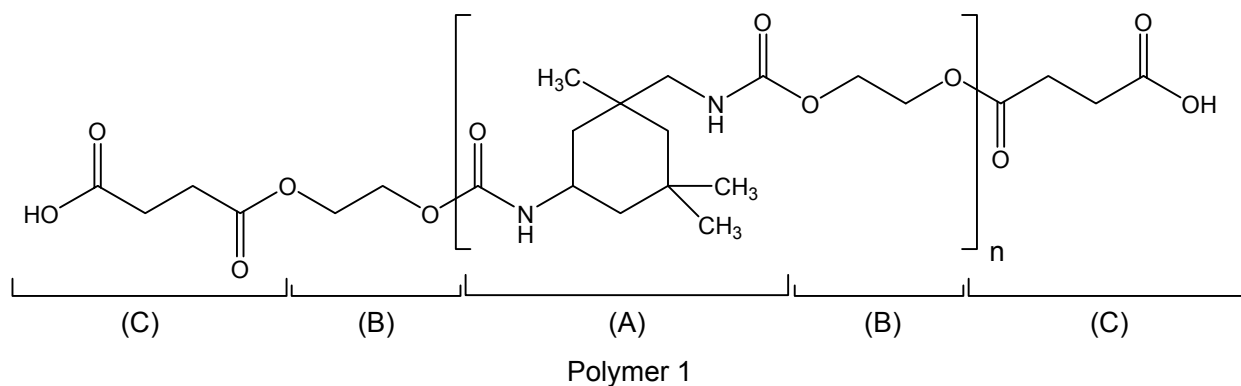
Example 1 - The reaction scheme to obtain Polymer 1 is:

STEP I – Polyurethane formation



STEP II – Esterification

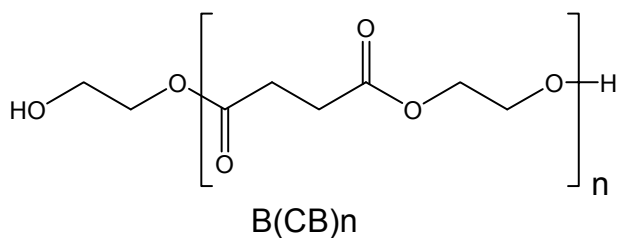
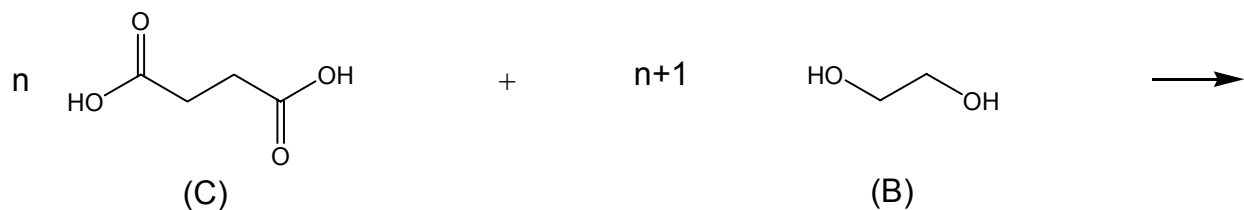




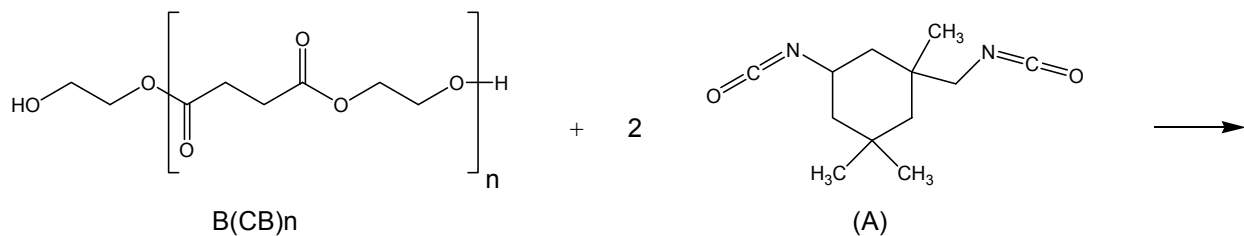
The final product, Polymer 1, has the structure $CB(AB)_n C$, where component C is derived from a diacid monomer. Because it does not contain reactive groups of concern, it may meet the RRR polymer criteria.¹

Example 2 - The reaction scheme to obtain Polymer 2 from the same three monomers is:

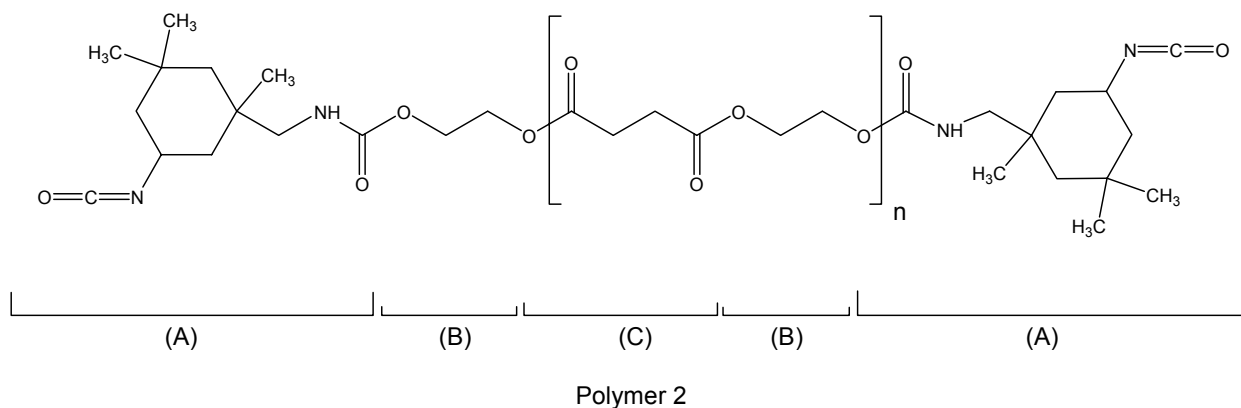
STEP I – Esterification



STEP II – Urethane formation



¹ For Polymer 1 to be deemed an RRR polymer, it must meet all other criteria indicated in Section 9 of the Regulations.



Polymer 2 has the structure $AB(CB)nA$ and contains unreacted isocyanates, which are reactive groups of concern. Therefore, this polymer may not meet the RRR polymer criteria.²

Reaction-Scheme Format

The reaction scheme includes both monomer and reactant information and a sequence description.

Item I: Monomer and Reactant Information

The notifier must provide a table of the chemical identities of all monomers, pre-polymers, and reactants along with their CAS Registry number, molecular weight (Mw), percent by weight (% by weight), and relative number of moles. Each monomer, pre-polymer, and reactant should be assigned an identifier for use in the sequence description.

Identifiers	Monomers and Reactants	CAS no.	Mw	% by weight	Relative no. of moles
A	Cyclohexane, 5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethyl-	4098-71-9	222	2.52	11
B	Poly(oxy-1,2-ethanediyl), α -hydro- ω -hydroxy-	25322-68-3	7850	97.22	12
C	Hexane, 1-isocyanato-	2525-62-4	127	0.002	2

² For Polymer 2 to be deemed an RRR polymer, it must meet all other criteria indicated in Section 9 of the Regulations.

Item II: Sequence Description

EITHER

- a) Provide the order and description of each step, including the nature of the reactions and the identifiers for all monomers, reactants, and intermediates. For example:

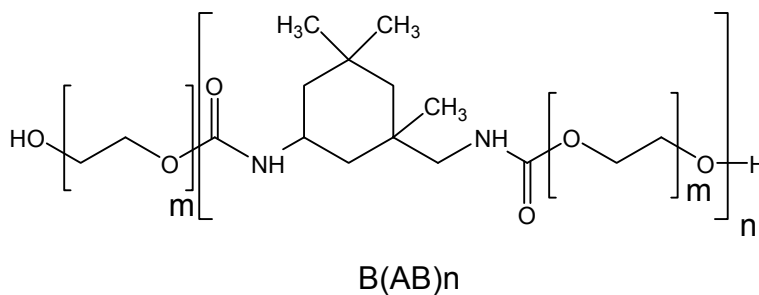
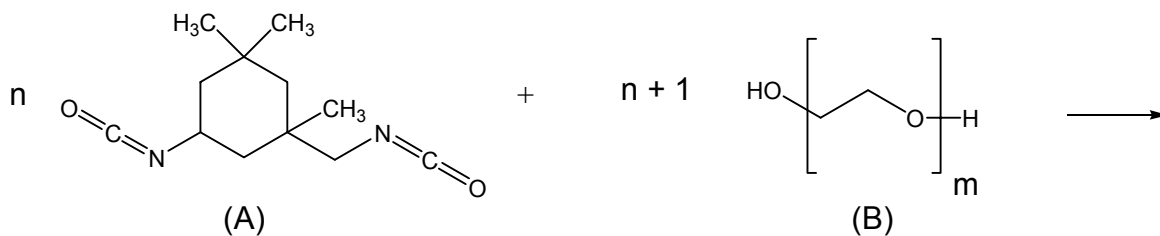
Step 1: $A + B \rightarrow$ Intermediate AB (*Polyurethane formation*)

Step 2: Intermediate AB + C \rightarrow Final Product (*Urethane end-cap formation*)

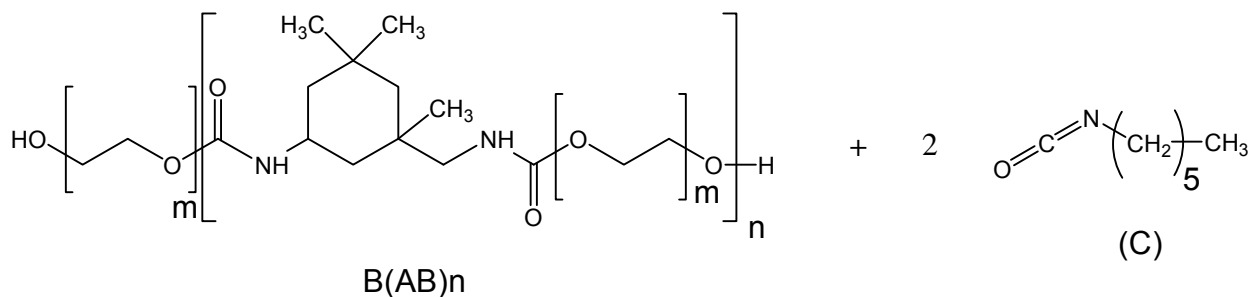
AND/OR

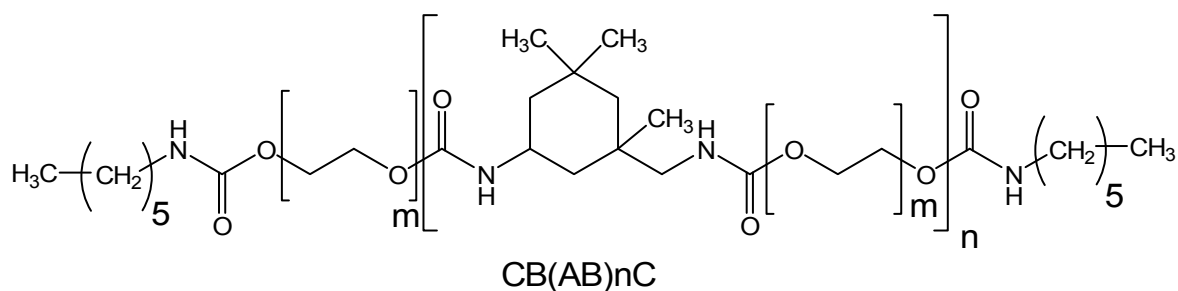
- b) Provide a sequencing description that uses structural formulae and includes the order and nature of the reactions and the identifiers for all monomers, reactants, and intermediates. For example:

STEP 1 – Polyurethane formation



STEP 2 – Urethane end-cap formation





$$m = 178 \quad n = 11$$

Other considerations

Exceptions

Under the Regulations, the reaction scheme is a mandatory information requirement for all RRR polymers that are notified under Schedule 9. However, if the notified substance meets the polyester-exemption criteria (paragraph 9(c) of the Regulations), a reaction scheme does not have to be submitted. Some polyester polymers are exempt if they are manufactured from a list of reactants outlined in Schedule 8 of the Regulations.

In addition, a reaction scheme is not required for non-RRR polymers.

Waivers

If a polymer meets the RRR polymer criteria for number-average molecular weight and oligomer content, and no functional groups of concern are present, the notifier may request a waiver of the reaction-scheme requirement under paragraph 81(8)(a) of the Act. The waiver request must be accompanied by an appropriate justification. Its acceptability will be evaluated by scientists from the New Substances Program.

Absent or Incomplete Reaction-Scheme Information

If a notifier is unable to submit a complete reaction scheme, there are two possible scenarios:

- a) The notifier may request a waiver for the reaction-scheme requirement if the polymer does not contain any functional groups of concern; or
- b) The New Substances Program will consider the polymer to have non-RRR status because its RRR status cannot be verified.

Please note that non-RRR status requires that additional information requirements must be met.

Foreign Supplier Submissions

If the notifier cannot access the reaction scheme because it is considered to be confidential by a foreign supplier, the information must be supplied directly to the New Substances Program by the Foreign Supplier. The confidential reaction scheme will be identified as a "Foreign Supplier Submission" (refer to Section 5.2 of the *Guidelines for the Notification and testing of New Substances: Chemicals and Polymers*, Version 2005 for further explanations).

Contact Information

New Substances Information Line

Telephone: 1-800-567-1999 (toll-free in Canada)
1-819-953-7156 (outside Canada)

Facsimile: 1-819-953-7155

E-mail: nsn-info@ec.gc.ca

For additional information or documentation regarding the New Substances Notification Regulations, please visit the New Substances Website at http://www.ec.gc.ca/substances/nsb/eng/index_e.htm.

Original signed by

Bernard Madé
Director
New Substances Division
Environment Canada

Signed on September 21, 2006