

Selectivity of the Isocyanate-Hydroxyl Reaction vs. Side Reactions as a Function of Catalysis

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POLYURETHANES IN COATINGS

-Reactive two components

Two package

Polyisocyanate + Polyol

One package

Blocked isocyanate +
Polyol

-Reactive one component

NCO prepolymer +
moisture; Oxidative

-Nonreactive one component

Solution

Thermoplastic PU

Aqueous solution

High and low MW PU

Thermoplastic and XL

ISOCYANATE REACTIONS

R-NCO

R-OH

R-NH₂

HOH

EPOXY

R-COOH

TRIMER

R-NHCONH-R

DIMER

R-NHCOO-R

CARBODIIMIDE

CATALYSIS PROBLEMS

HIGH SOLIDS COATINGS

**POTLIFE/REACTIVITY
MOISTURE REACTION
SOLUBILITY
NETWORK STABILITY**

WATERBORNE

**WATER REACTION
POTLIFE
GASING
STABILITY
GLOSS**

Objectives of this Study

ENVIRONMENTALLY ACCEPTABLE CATALYSTS

REACTION RATE OF CATALYSTS WITH OH

SELECTIVE CATALYSTS FOR OH

IMPROVED POTLIFE/REACTIVITY

REDUCED WATER REACTION

CATALYSTS USED

DIBUTYLTIN DILAURATE/DIACETATE

DIBUTYLTIN OXIDE

AMINES

LEAD COMPOUNDS

ZINC SALTS

MANGANESE SALTS

CATALYST PROPERTIES

POTLIFE / REACTIVITY

SELECTIVITY

DELAYED ACTION

LOW TEMPERATURE

HIGH TEMPERATURE

WATER

HIGH RATE (RIM)

EXTERIOR DURABILITY

RESISTANCE PROPERTIES

ENVIRONMENT - TOXICITY

Isocyanate-Hydroxyl Reactions

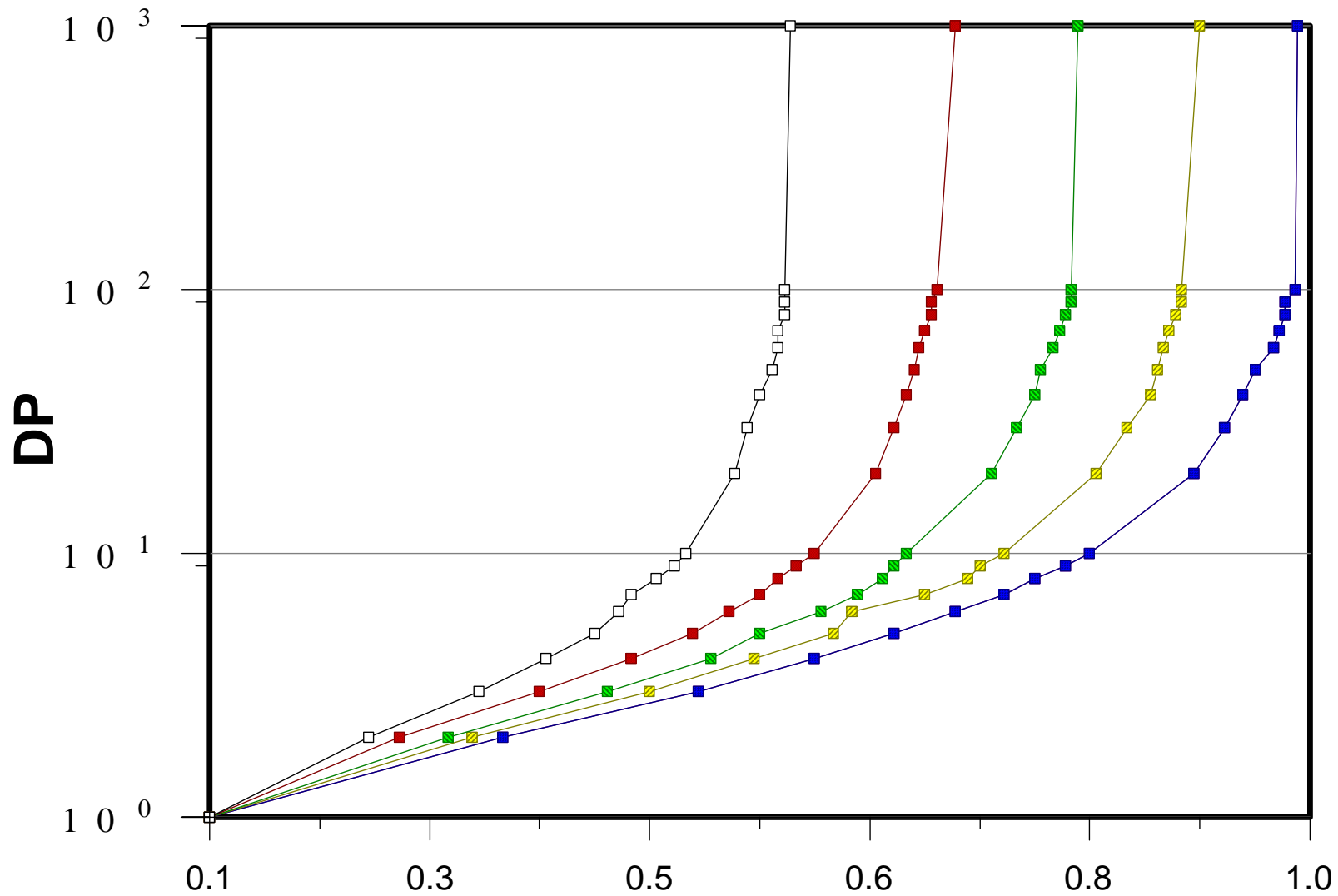


ADDITIONAL REACTIONS



MW AS A FUNCTION OF CONVERSION

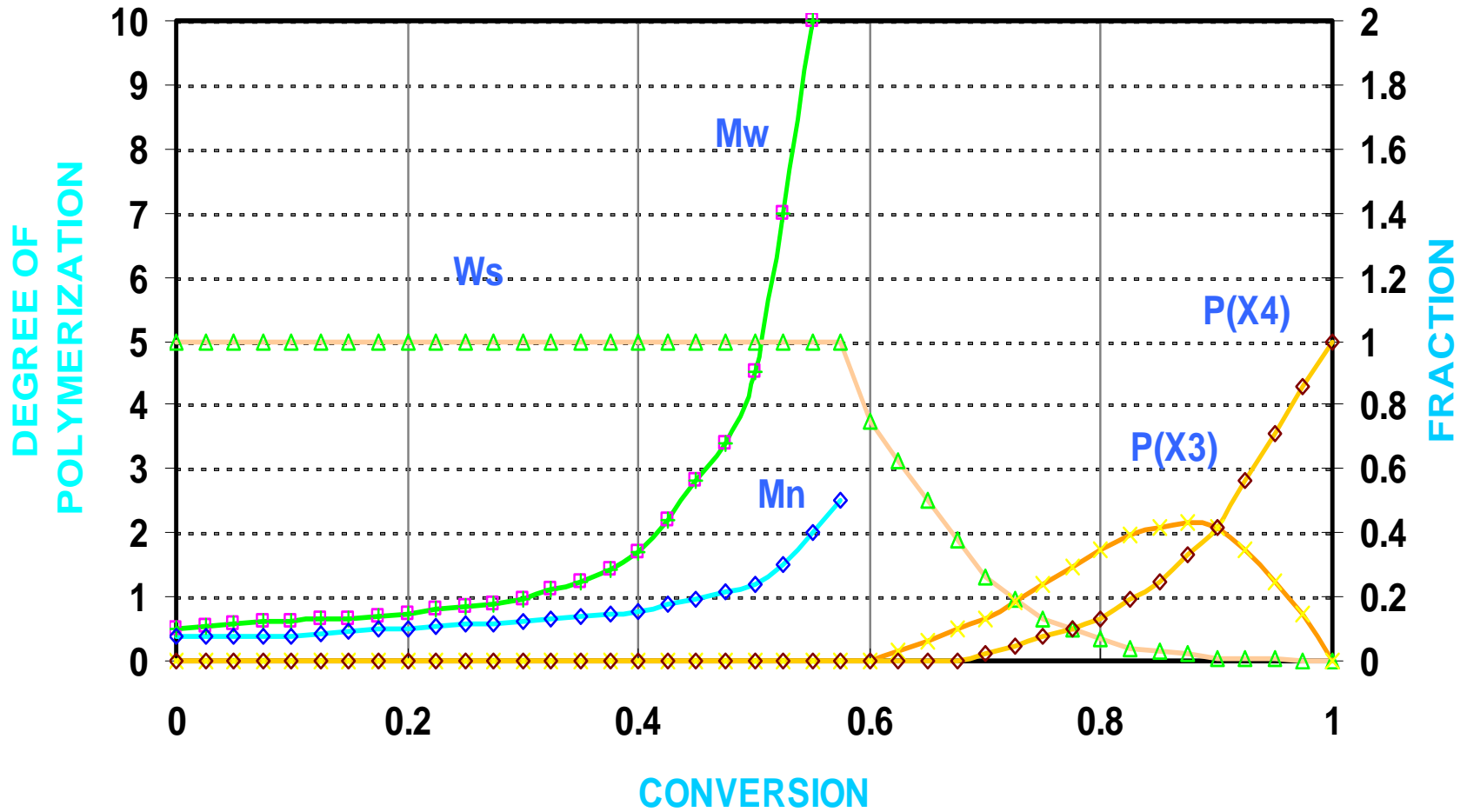
CROSSLINKER DIFUNCTIONAL



Note: This is a sub-note.

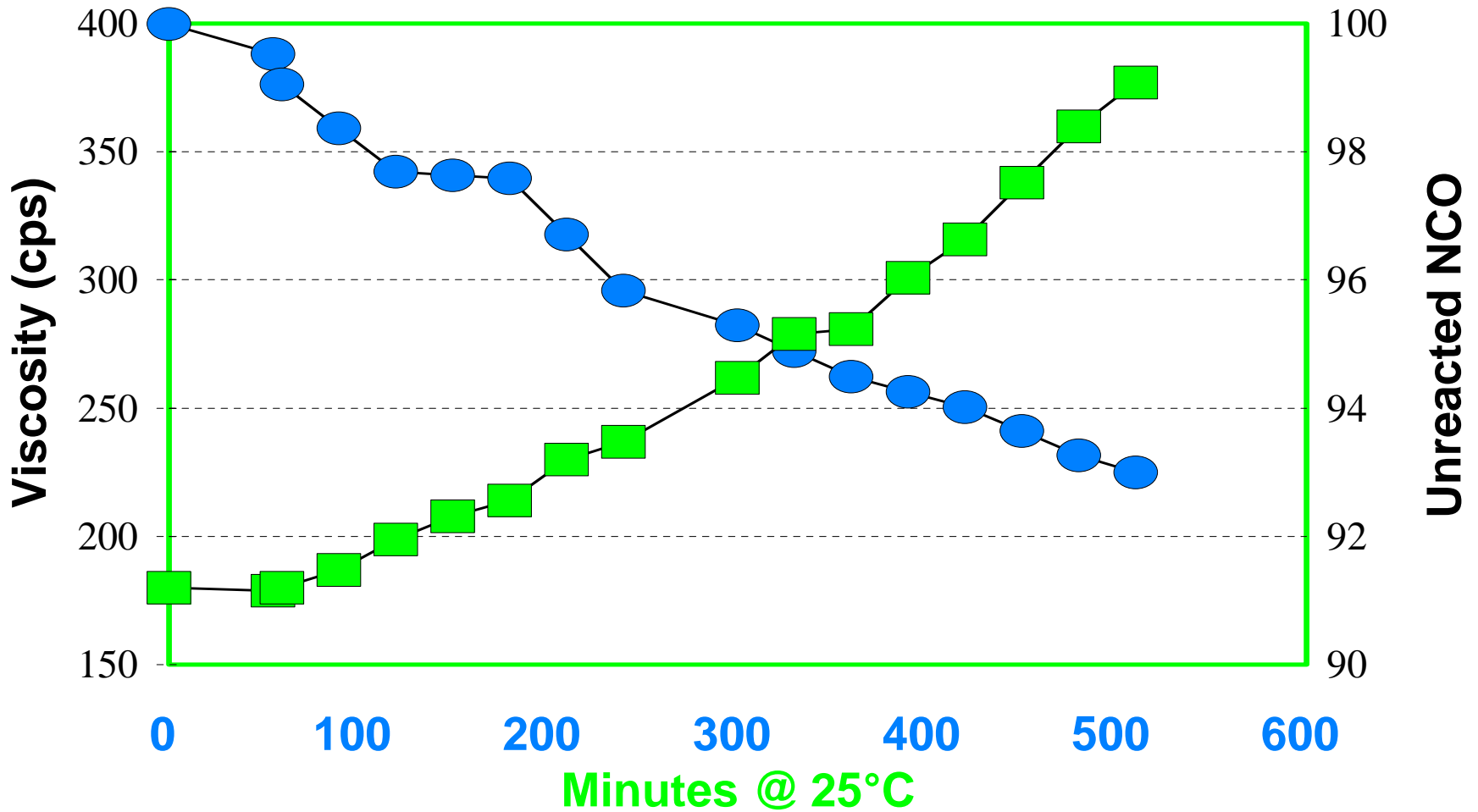
Conversion

NETWORK FORMATION A4 + B2



PE/HDI-TRIMER

No Catalyst



● % NCO

■ VISCOSITY

SL2017

SCREENING OF CATALYSTS

APPLICATION TESTS FORMULATION

POTLIFE (2X VISC.

GEL TIME

TACK FREE

DRY-THROUGH

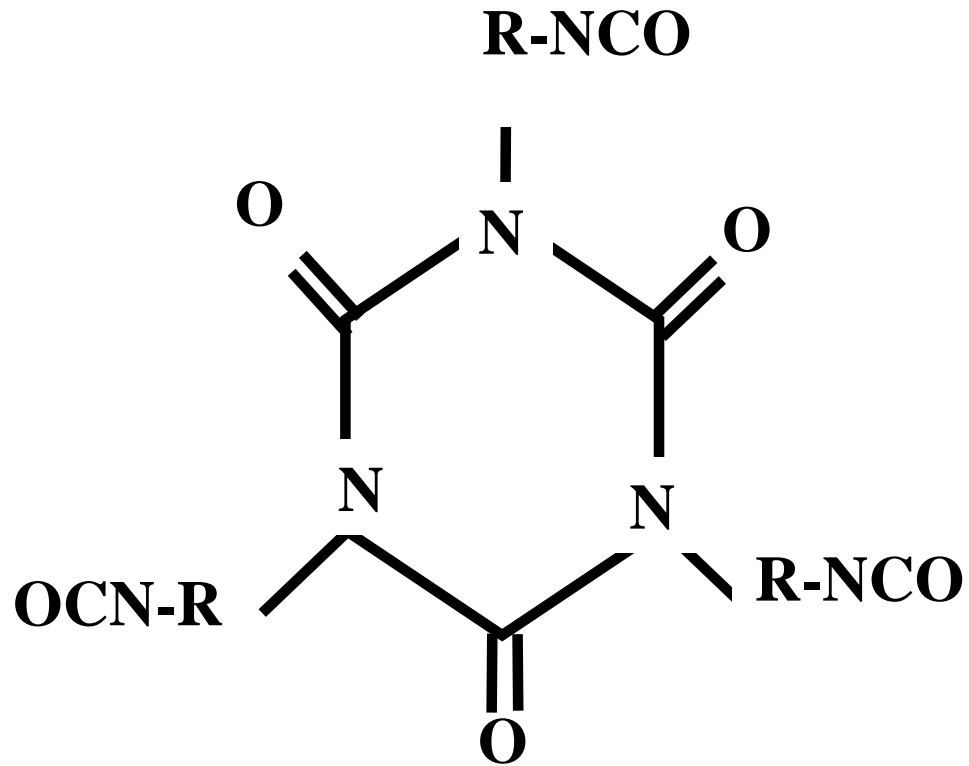
MODEL SYSTEMS (ANALYTICAL)

DISAPPEARANCE OF NCO

FORMATION OF URETHANE / UREA

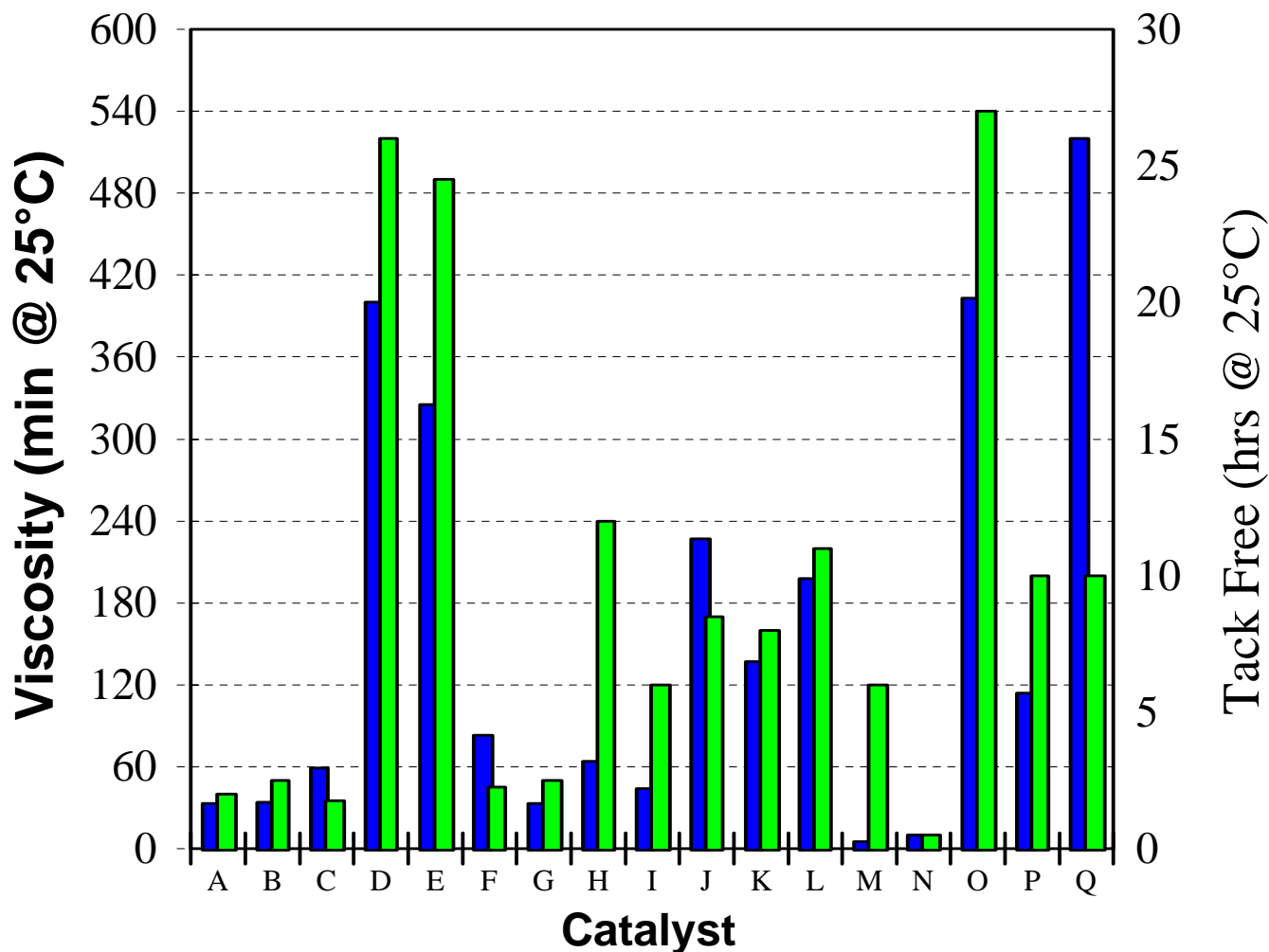
MW

HDI-TRIMER



Catalyst Study (HDI TRIMER)

Metal (0.0065% on Solids)



- A: DBTDL
- B: DBTDA
- C: Mn Naph/PD
- D: Mn Oct
- E: Sn Oct/PD
- F: Vn acac/PD
- G: Vn acac
- H: Bi Oct
- I: Bi Naph
- J: Zn acac/PD
- K: Zn Oct
- L: Co Oct
- M: Zr acac
- N: Zr acac/PD
- O: Zr Oct
- P: Al acac
- Q: Al chelate/PD



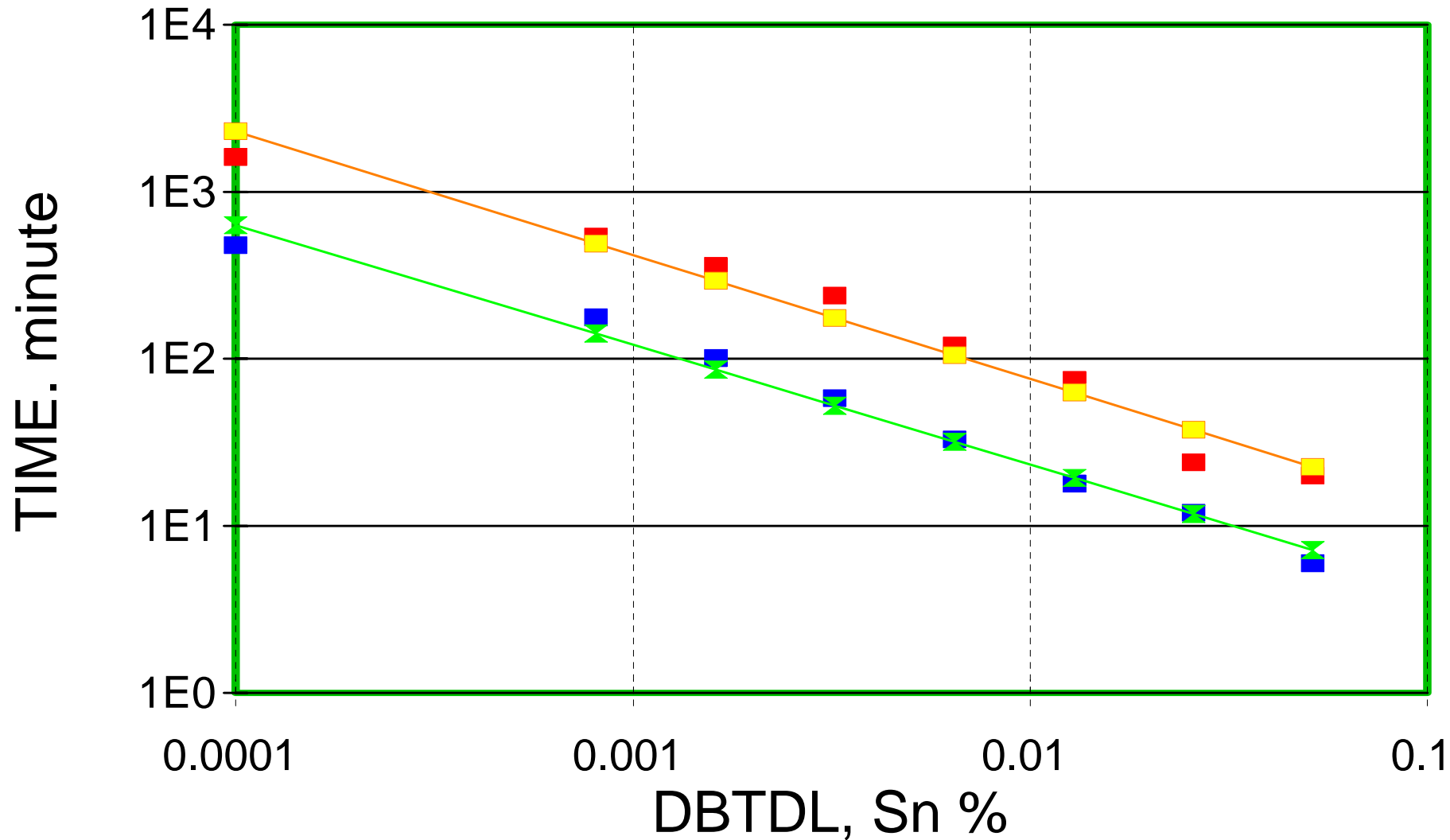
VISC. 2X



Tack Free (hrs)

PE/HDI-TRIMER

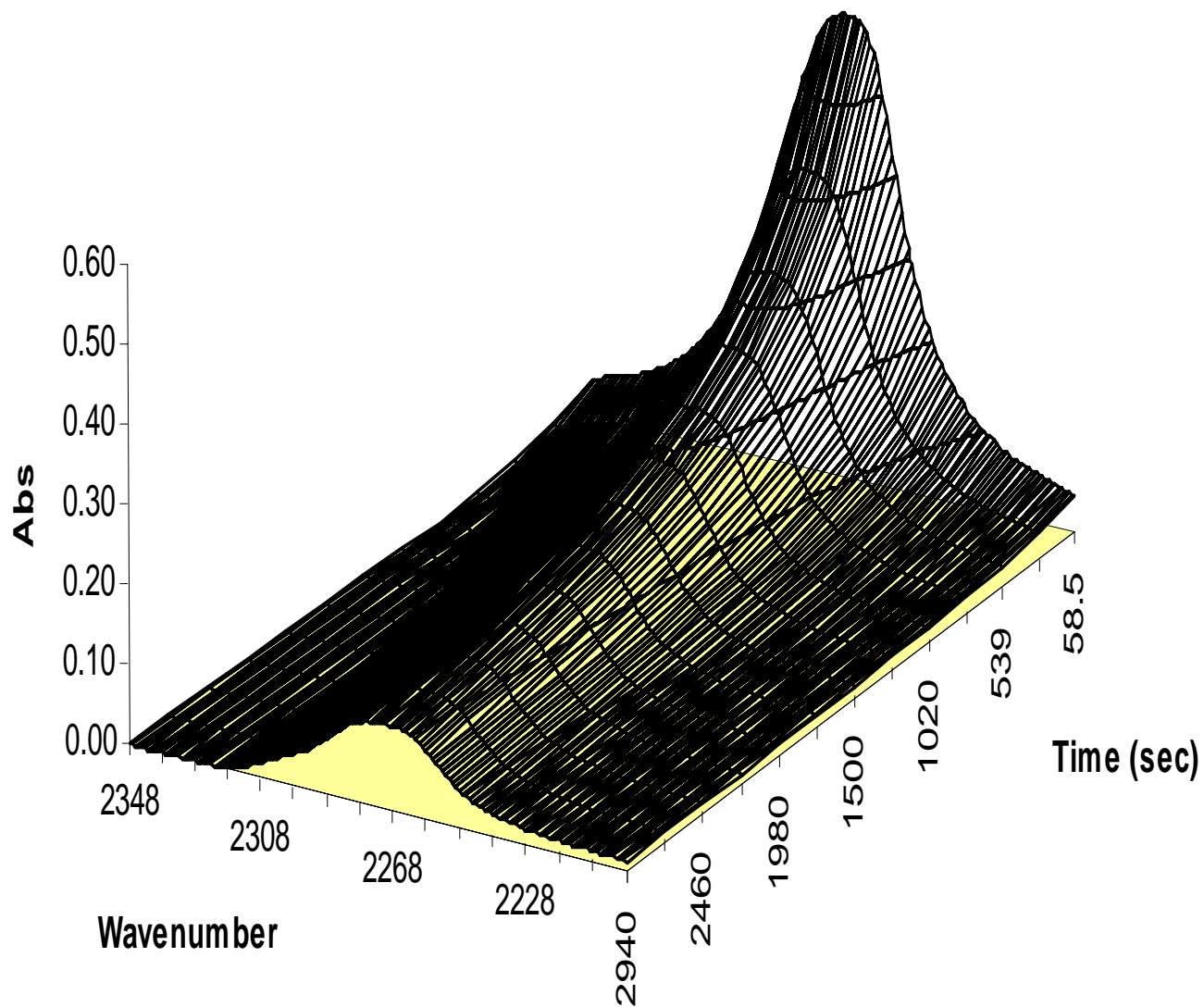
CATALYST REACTION RATE



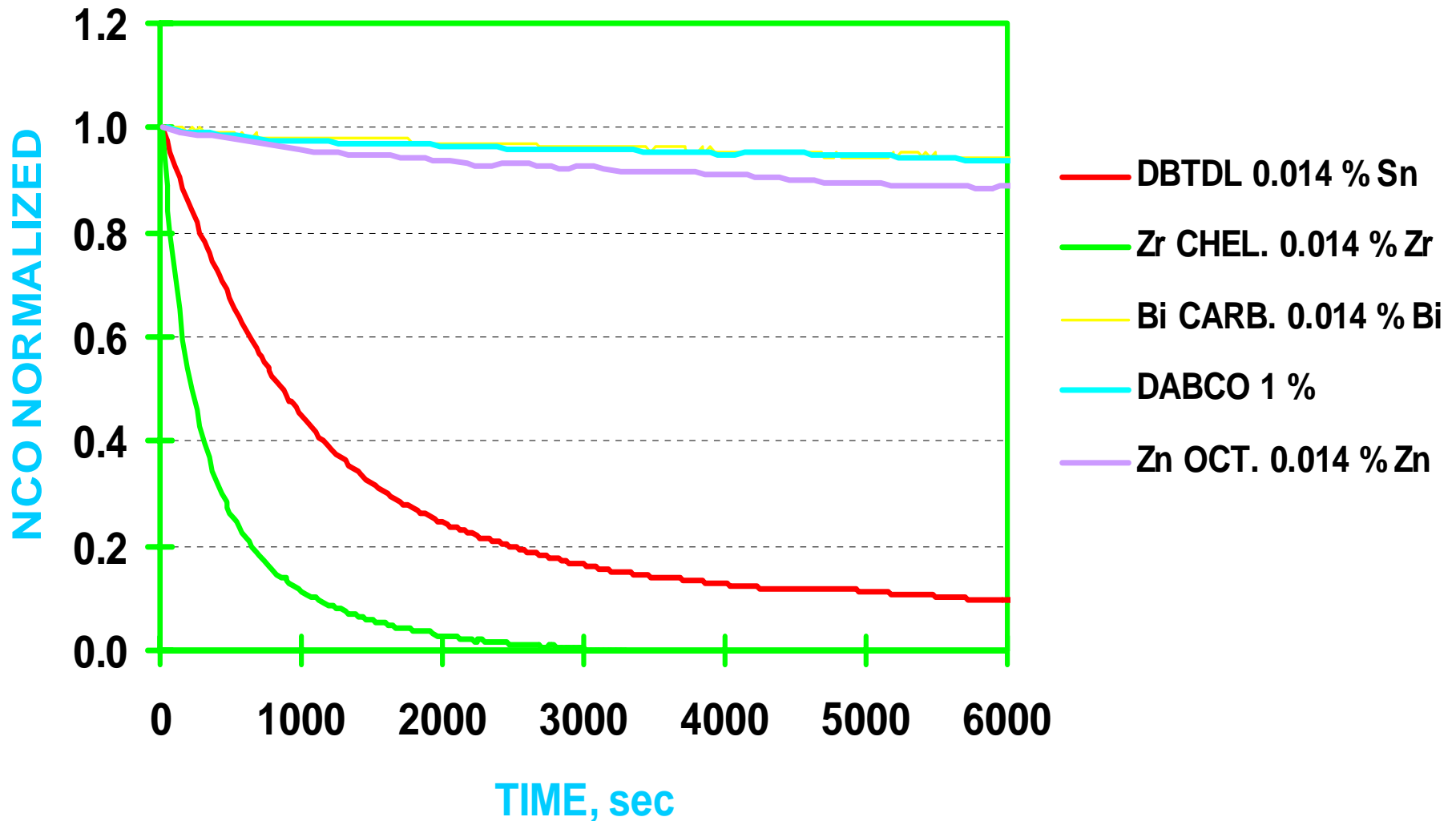
—△— Potlife

—□— TACK FREE

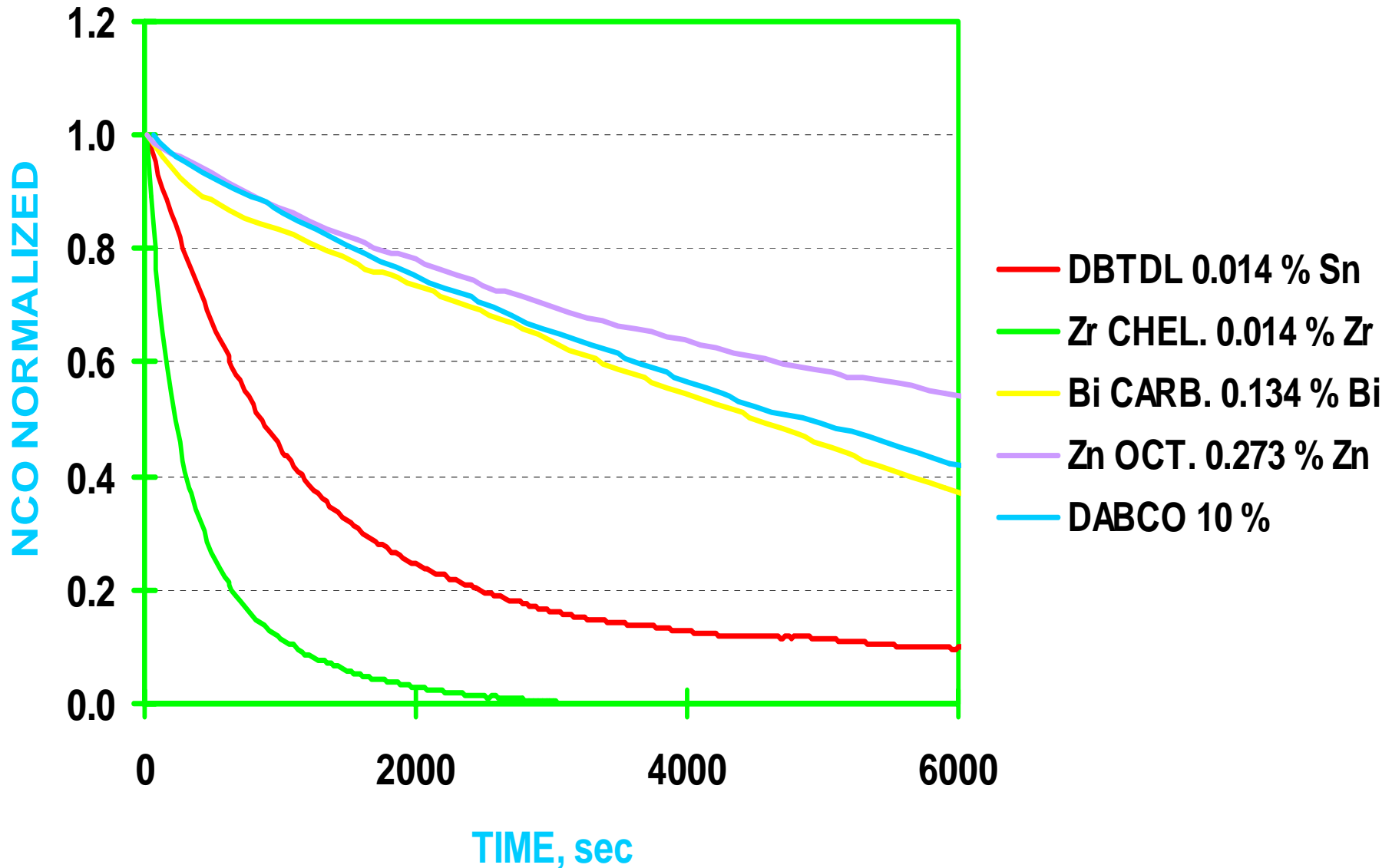
Isocyanate Peak Decay



HDI TRIMER / HYDROXYL
DBTDL 0.0140% Sn
n-BUTANOL

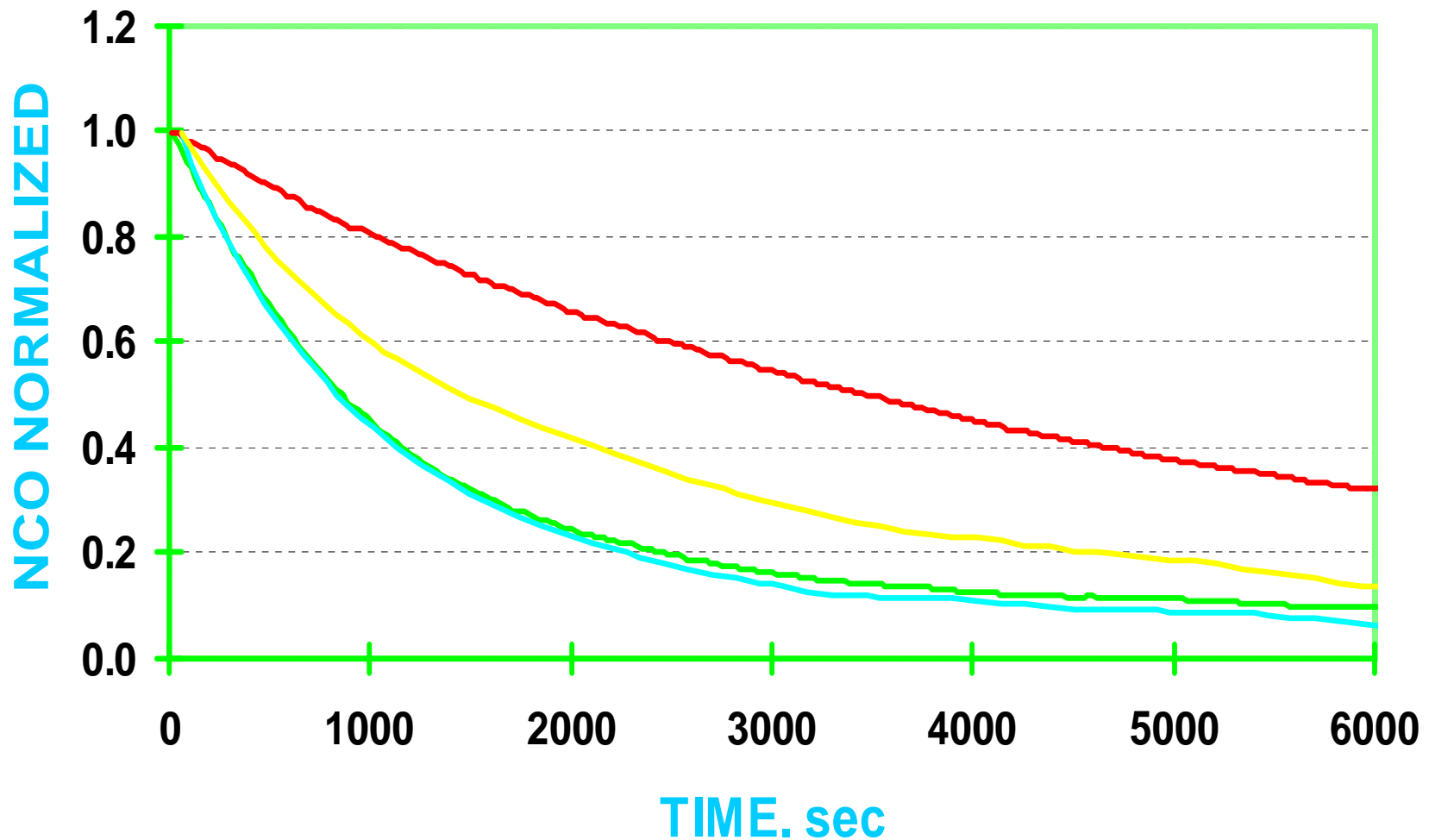


HDI TRIMER / n-BUTANOL



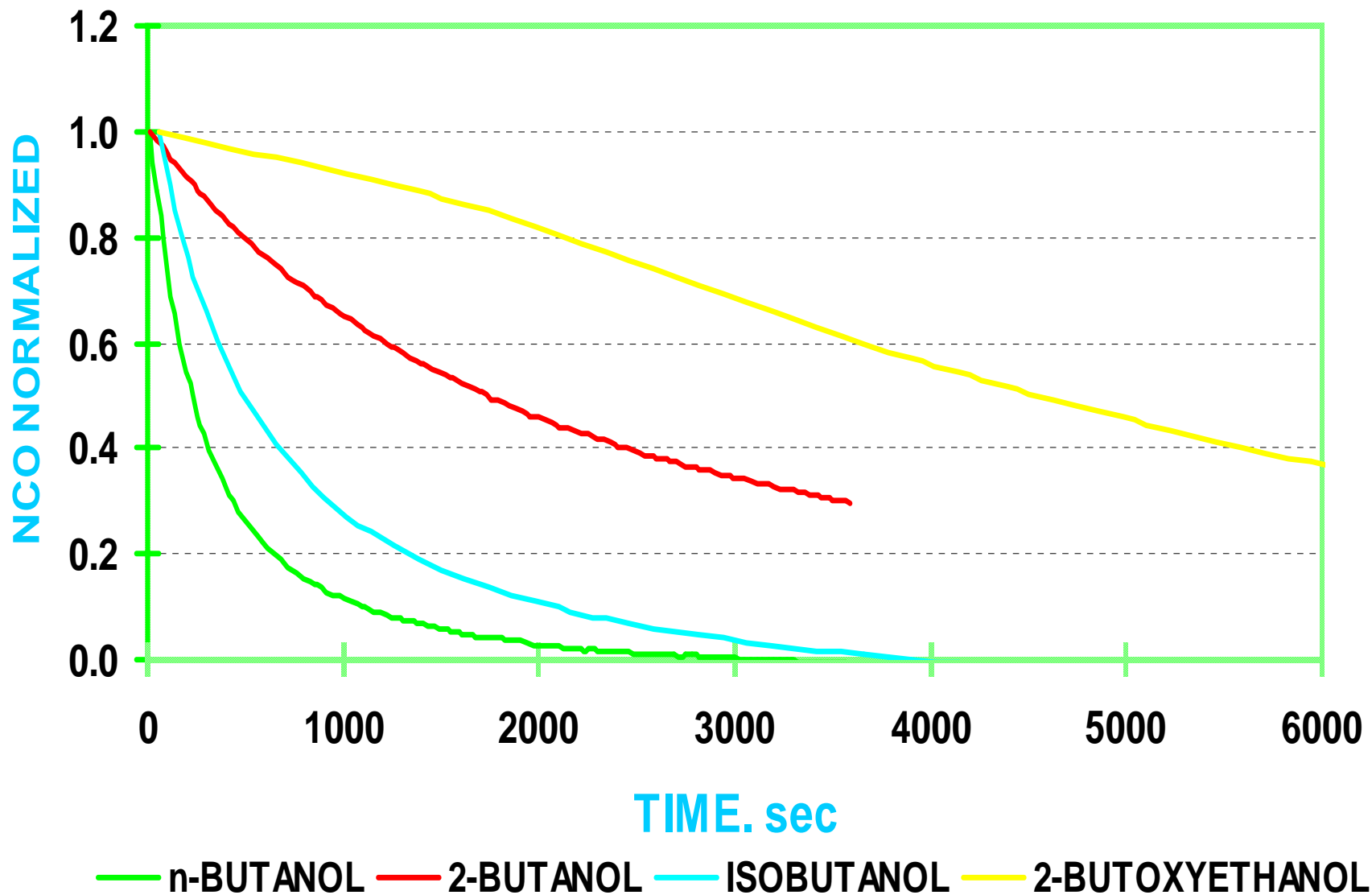
HDI-TRIMER - HYDROXYL

DBTDL 0.014% Sn

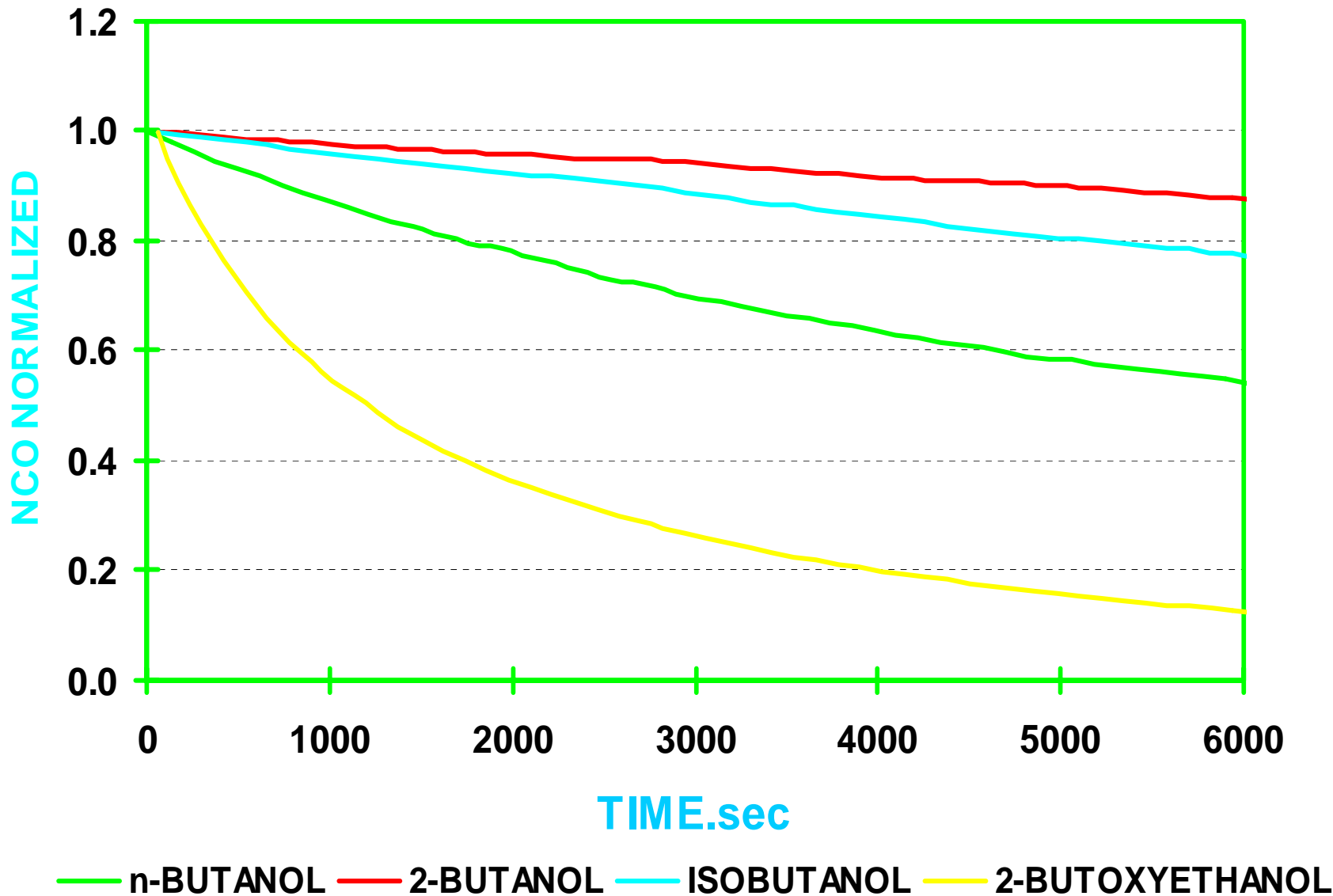


— n-BUTANOL — 2-BUTANOL — ISOBUTANOL — 2-BUTOXYETHANOL

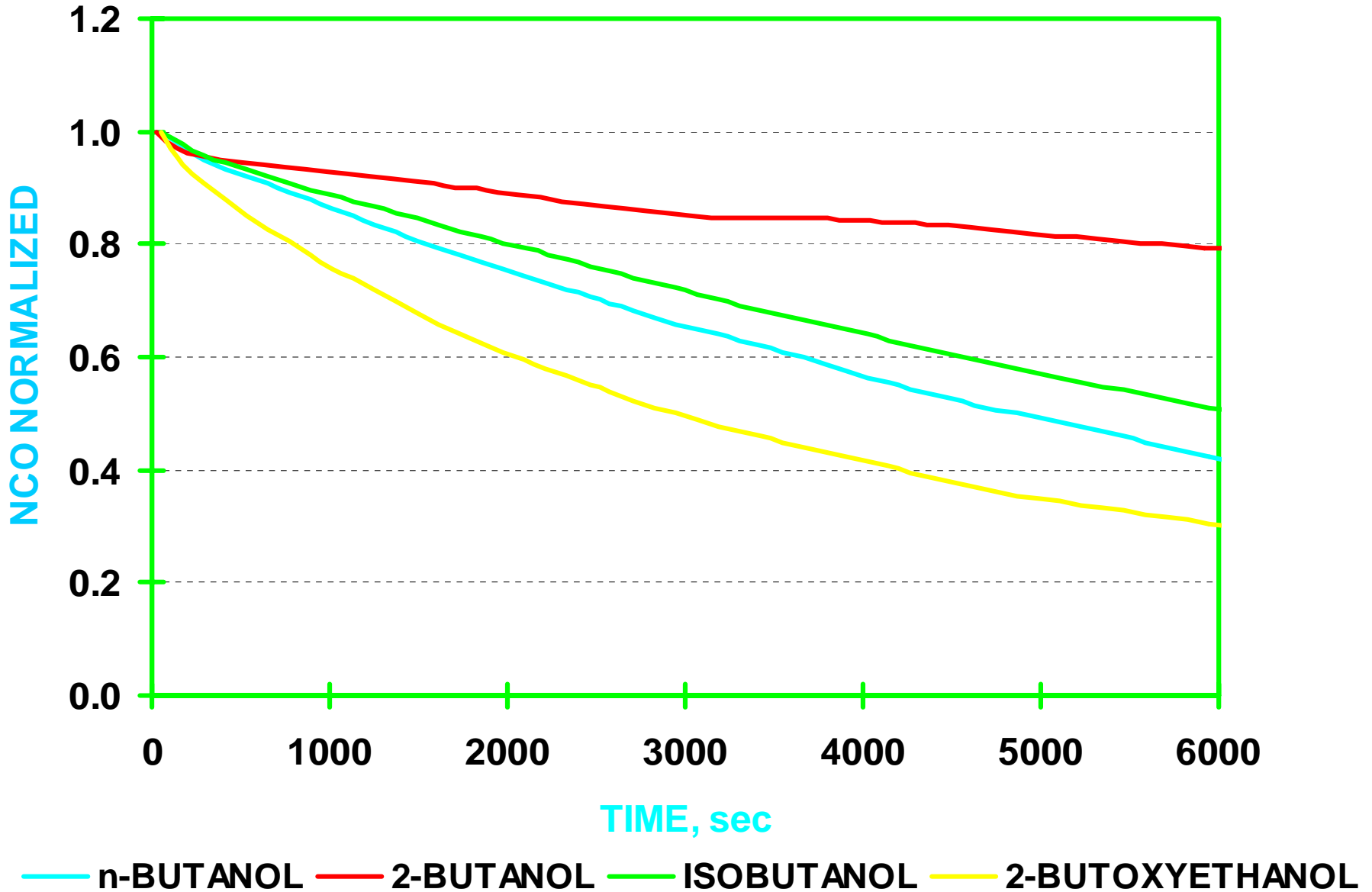
HDI TRIMER / HYDROXYL
Zr CHELATE 0.014% Zr



HDI TRIMER / HYDROXYL
Zn OCTOATE 0.272% Zn

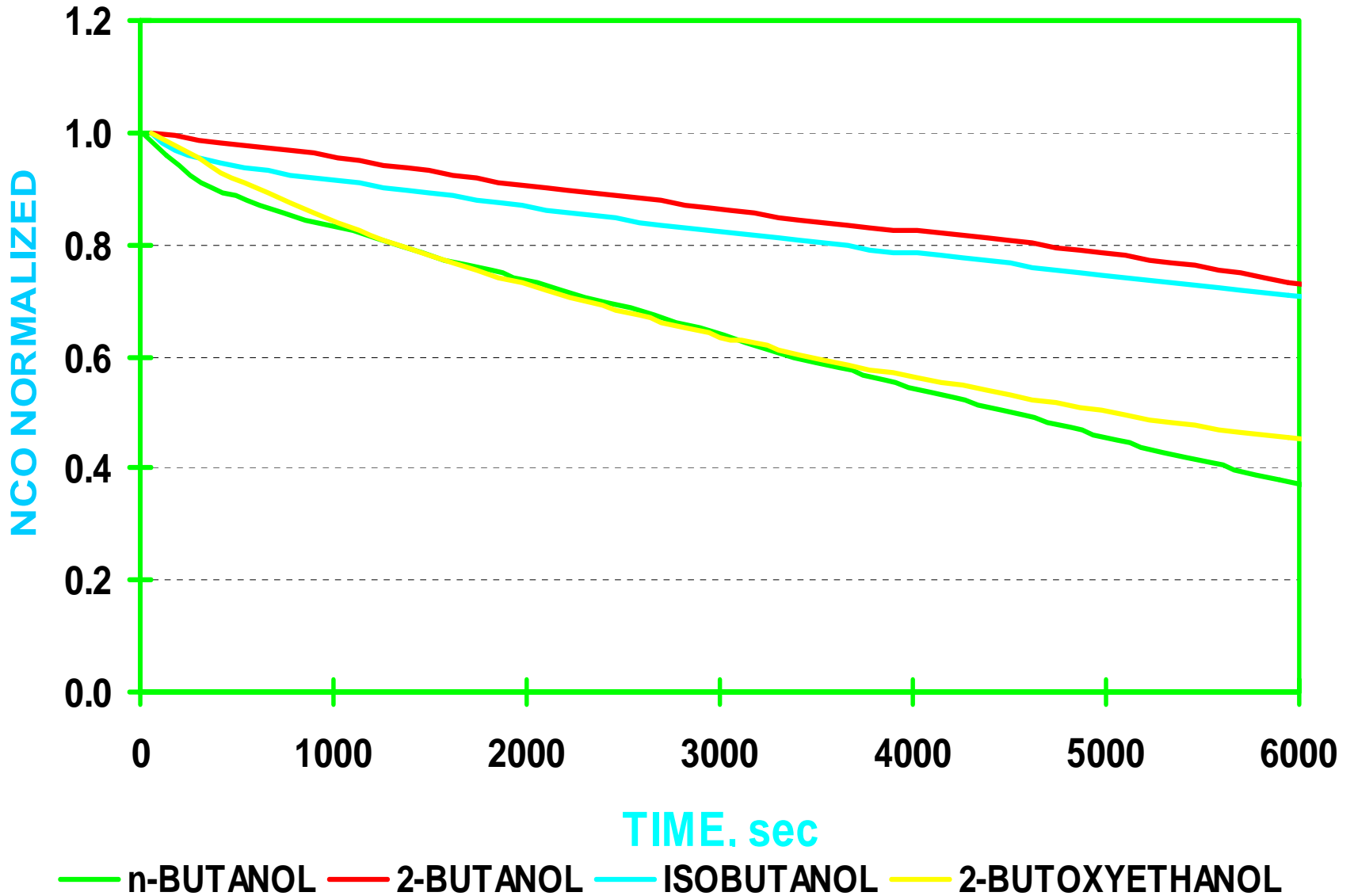


HDI TRIMER / HYDROXYL DABCO 10%



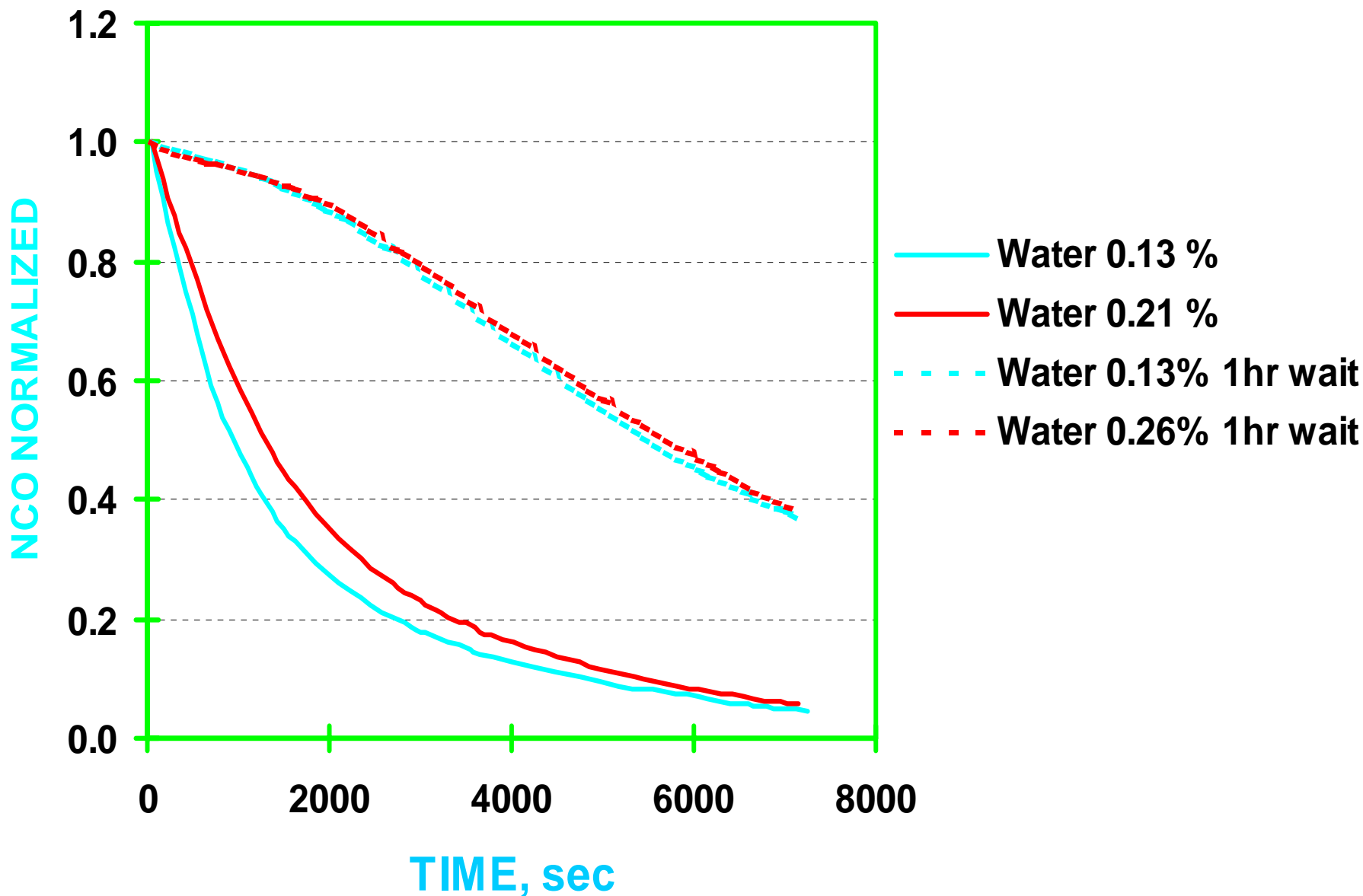
HDI TRIMER / HYDROXYL

Bi CARB. 0.134 % Bi

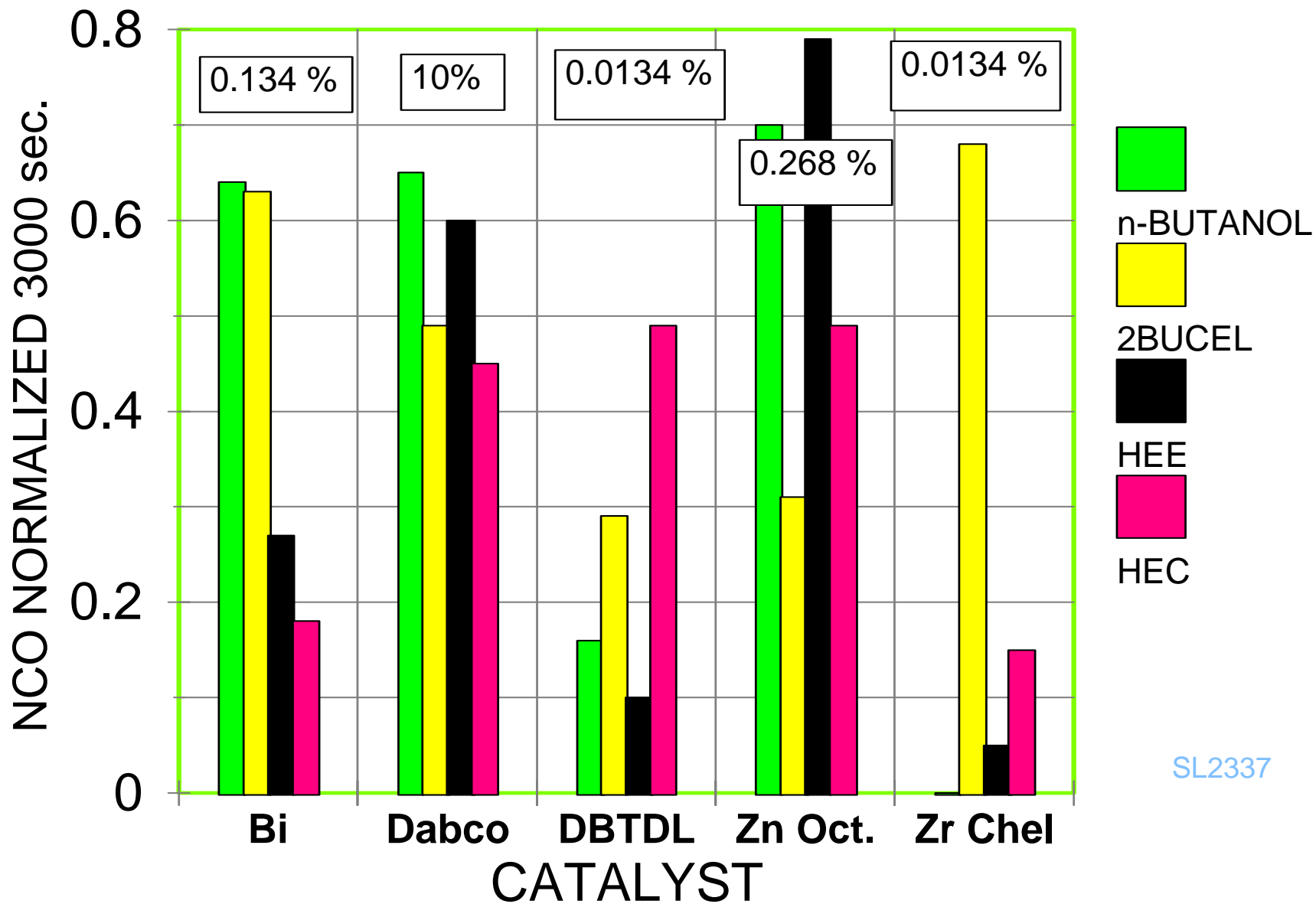


HDI TRIMER / 2-BUTOXYETHANOL

Zr CHELATE 0.028 % Zr, WATER EFFECT

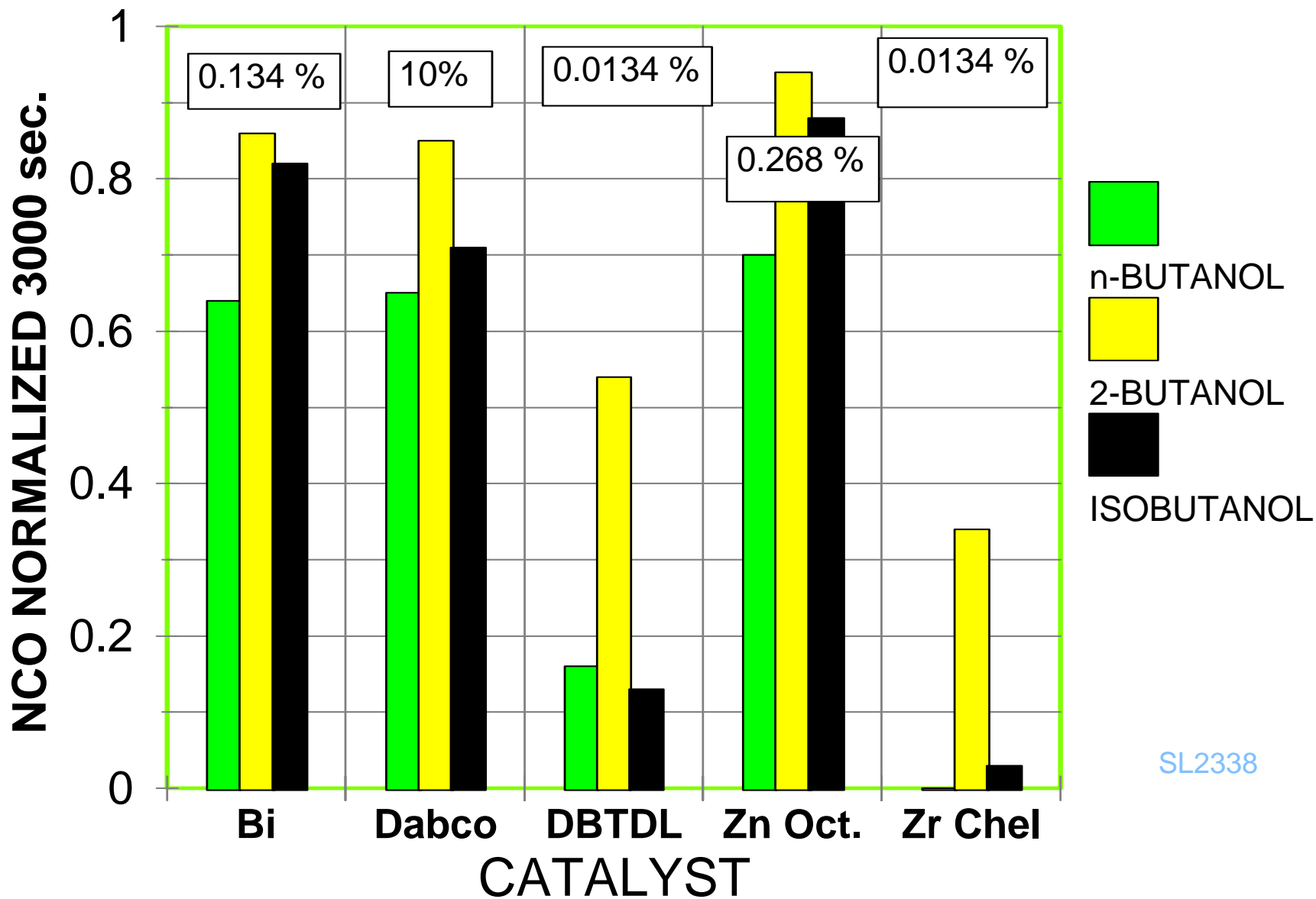


HDI-TRIMER/HYROXYL PRIMARY HYDROXL



HDI-TRIMER/HYROXYL

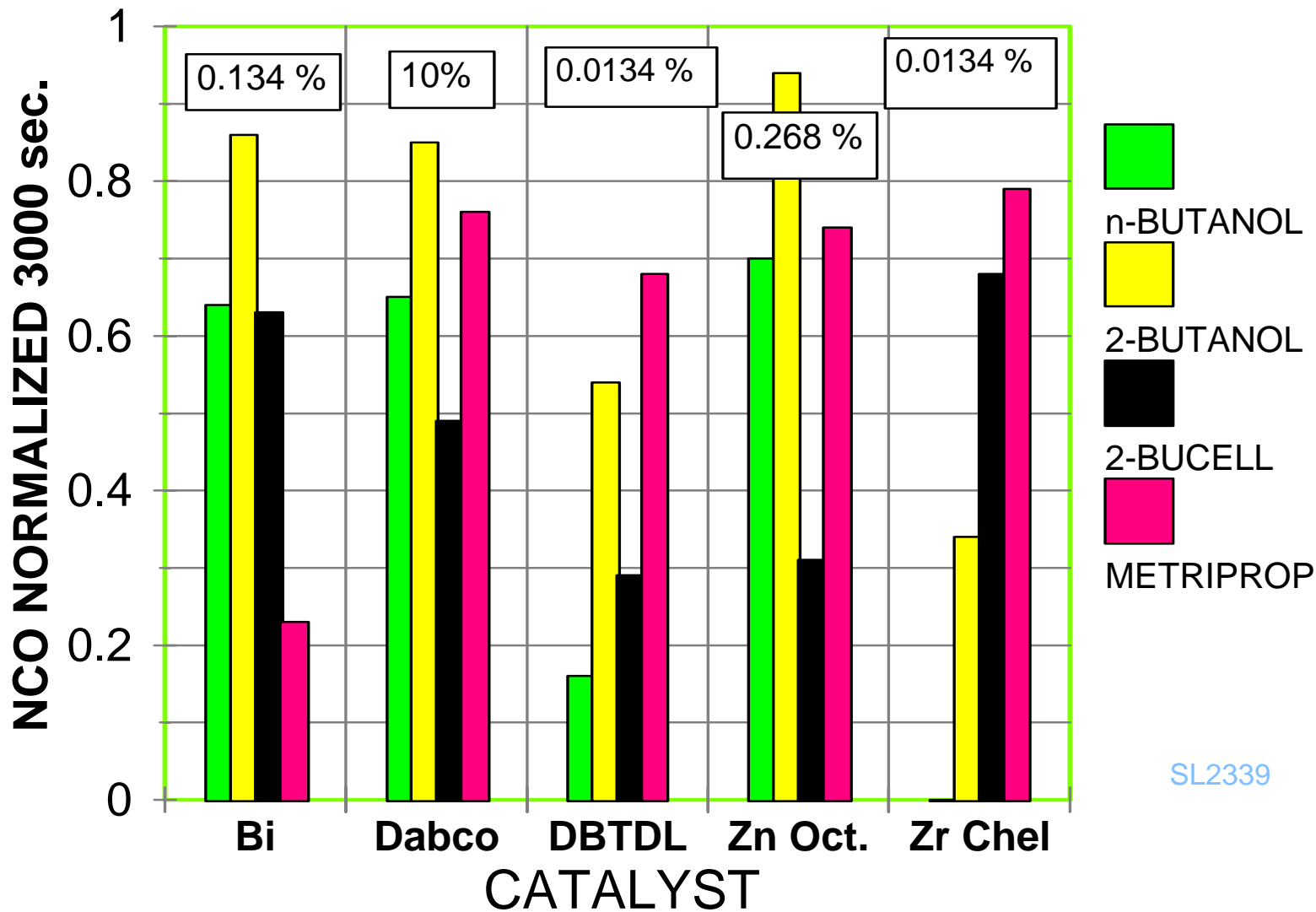
pri, sec BUTANOL



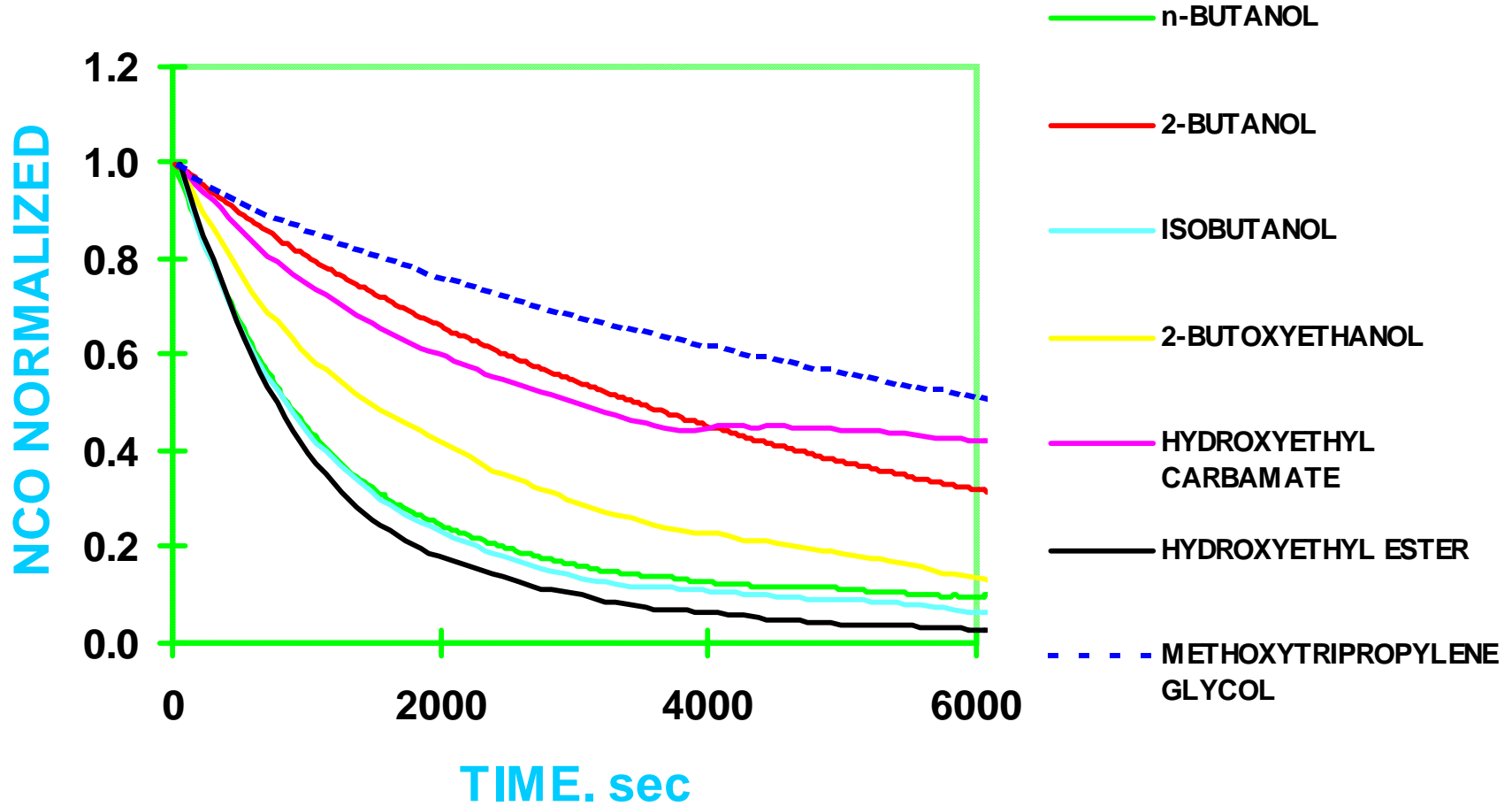
SL2338

HDI-TRIMER/HYROXYL

pri, sec BUTANOL, ETHER

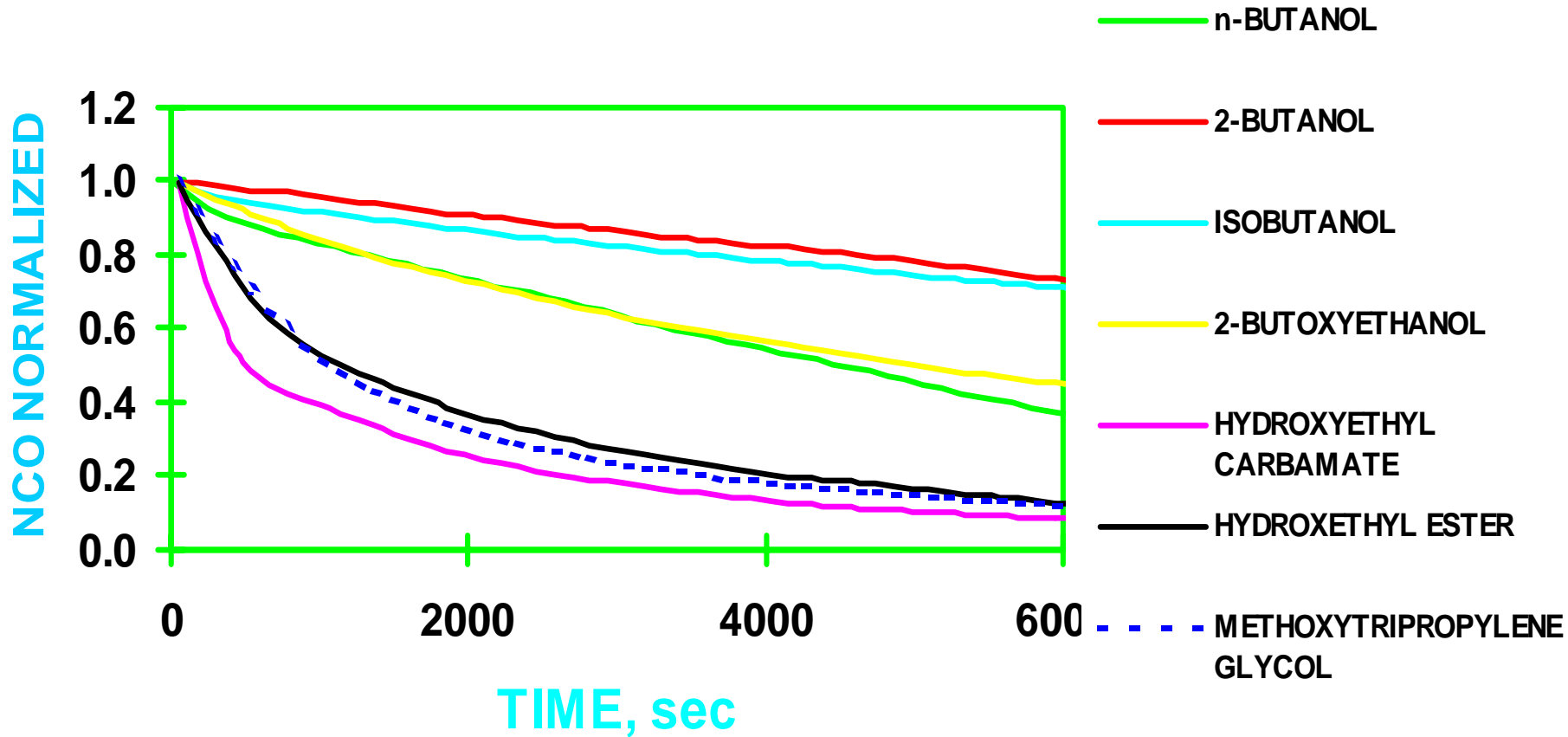


HDI-TRIMER - HYDROXYL DBTDL 0.014% Sn



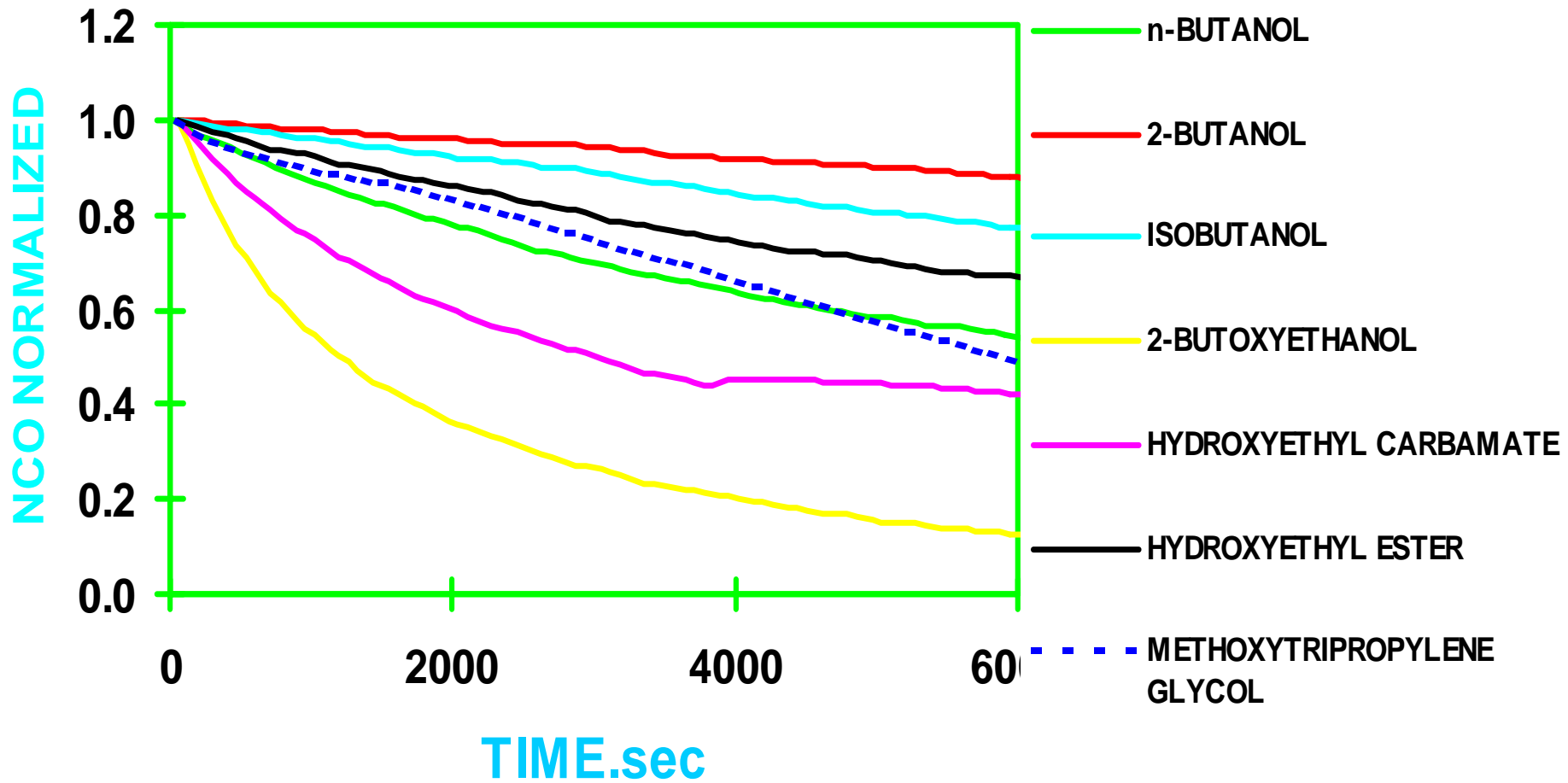
SL2340

HDI TRIMER / HYDROXYL Bi CARB. 0.134 % Bi



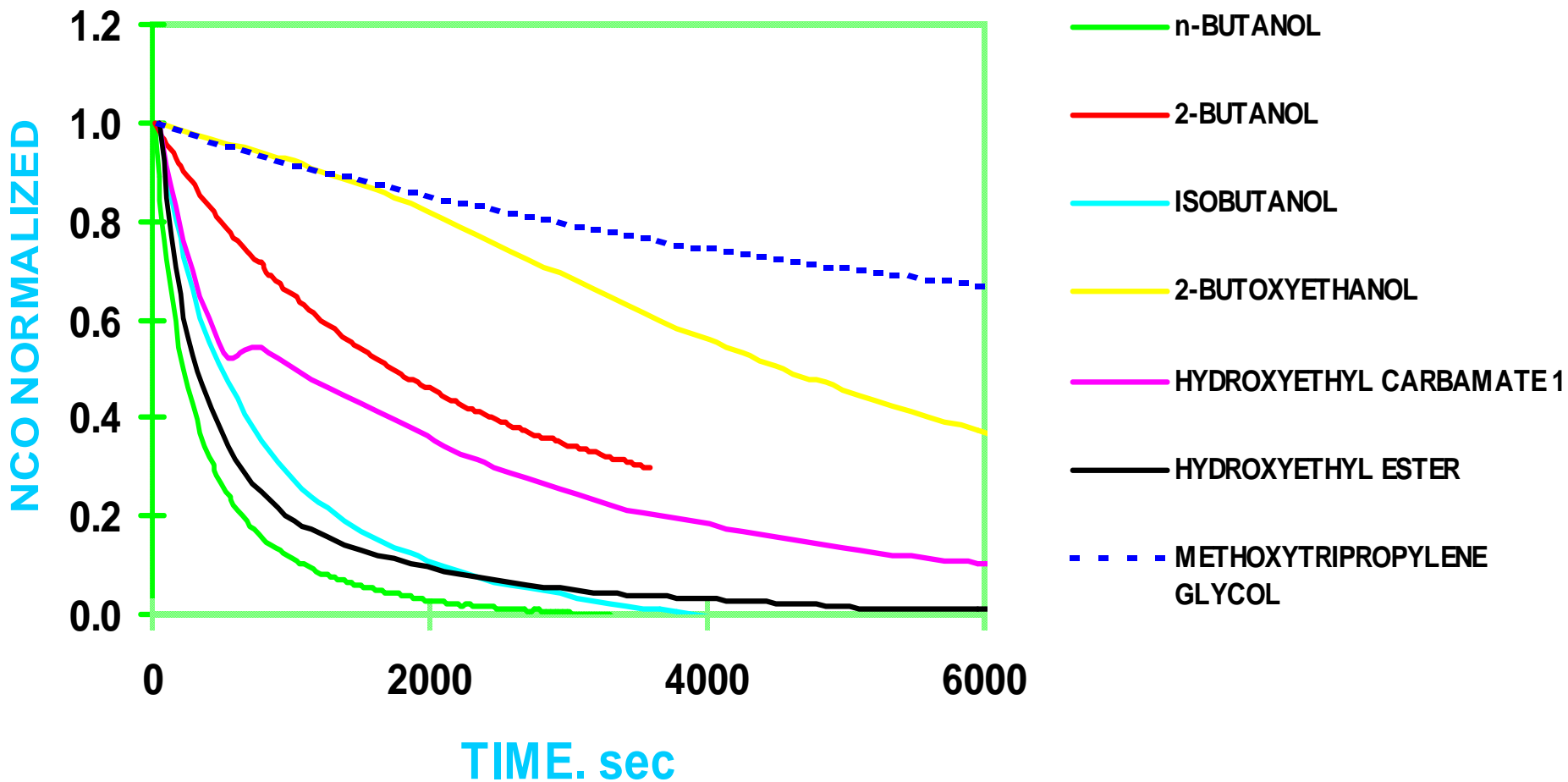
SL2341

HDI TRIMER / HYDROXYL Zn OCTOATE 0.272% Zn



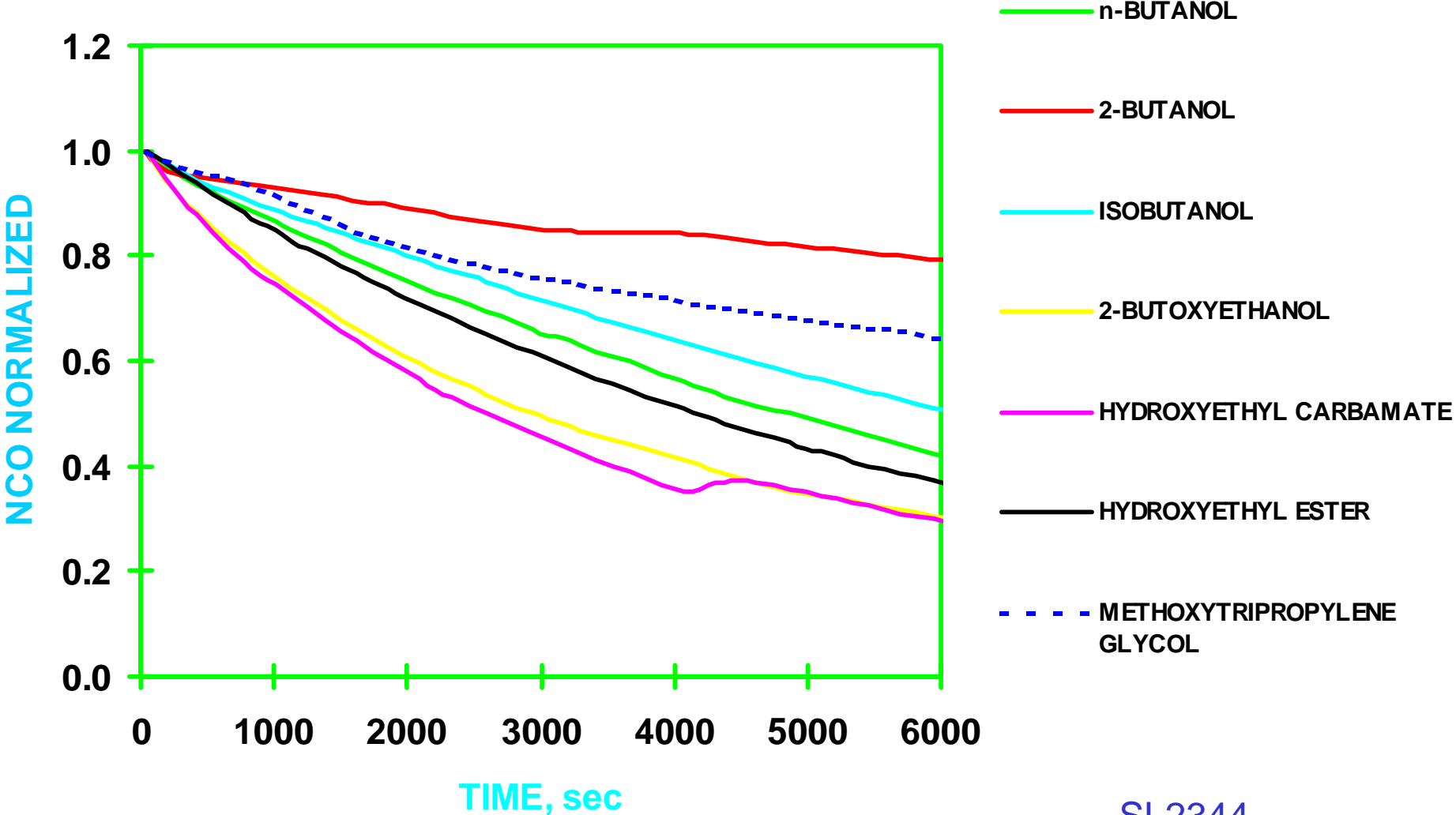
SL2342

HDI TRIMER / HYDROXYL Zr CHELATE 0.014% Zr



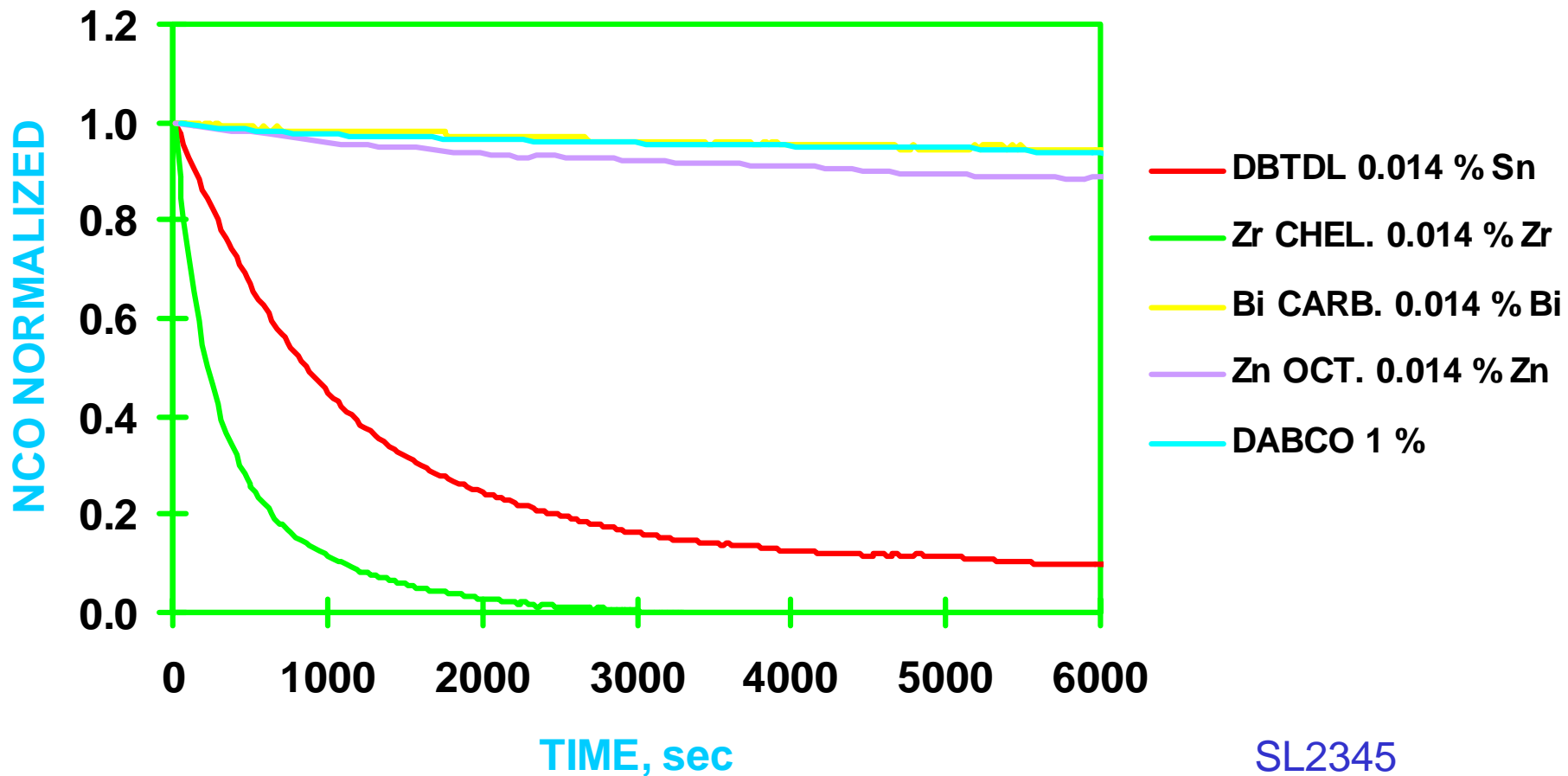
SL2343

HDI TRIMER / HYDROXYL DABCO 10%



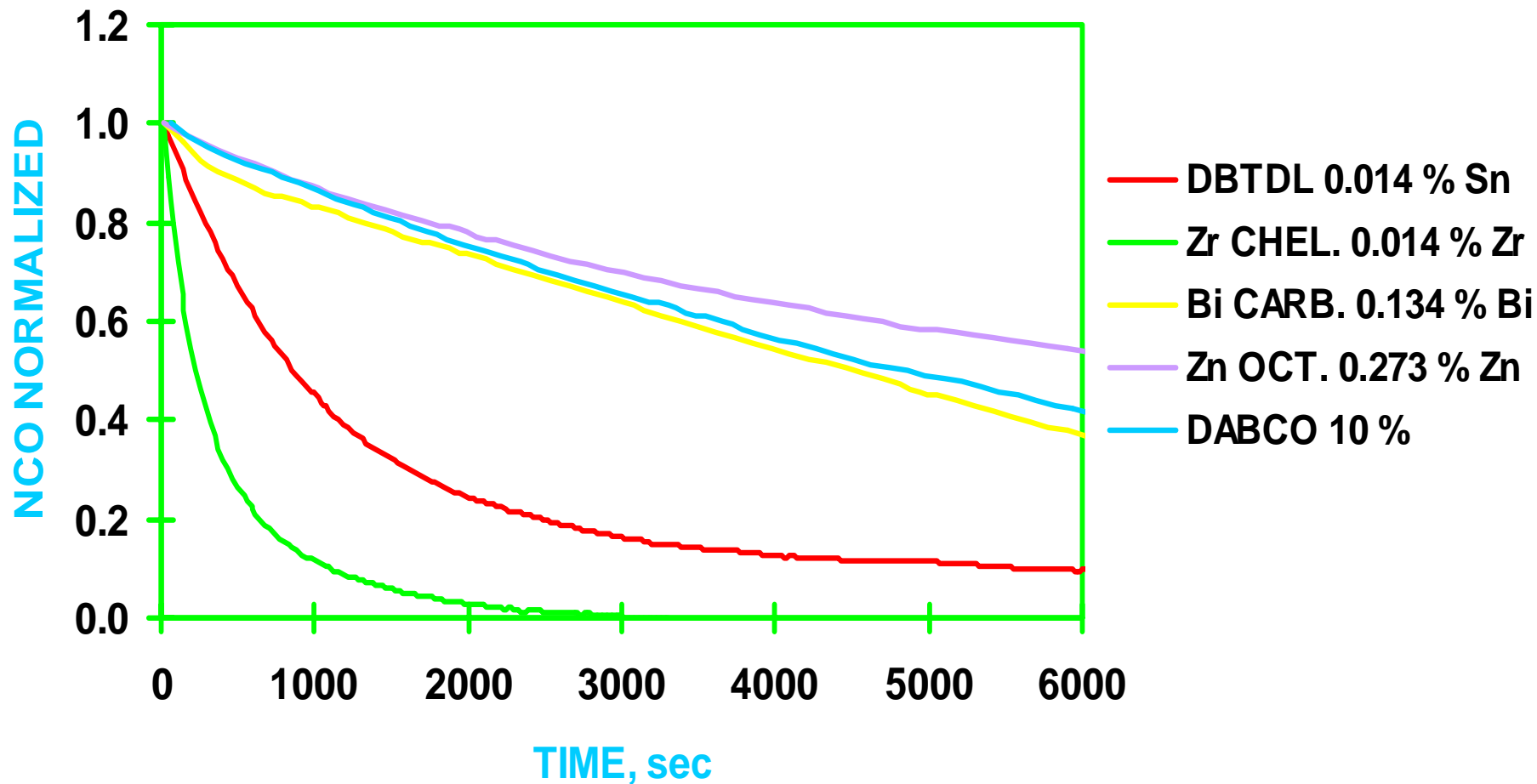
SL2344

HDI TRIMER / n-BUTANOL



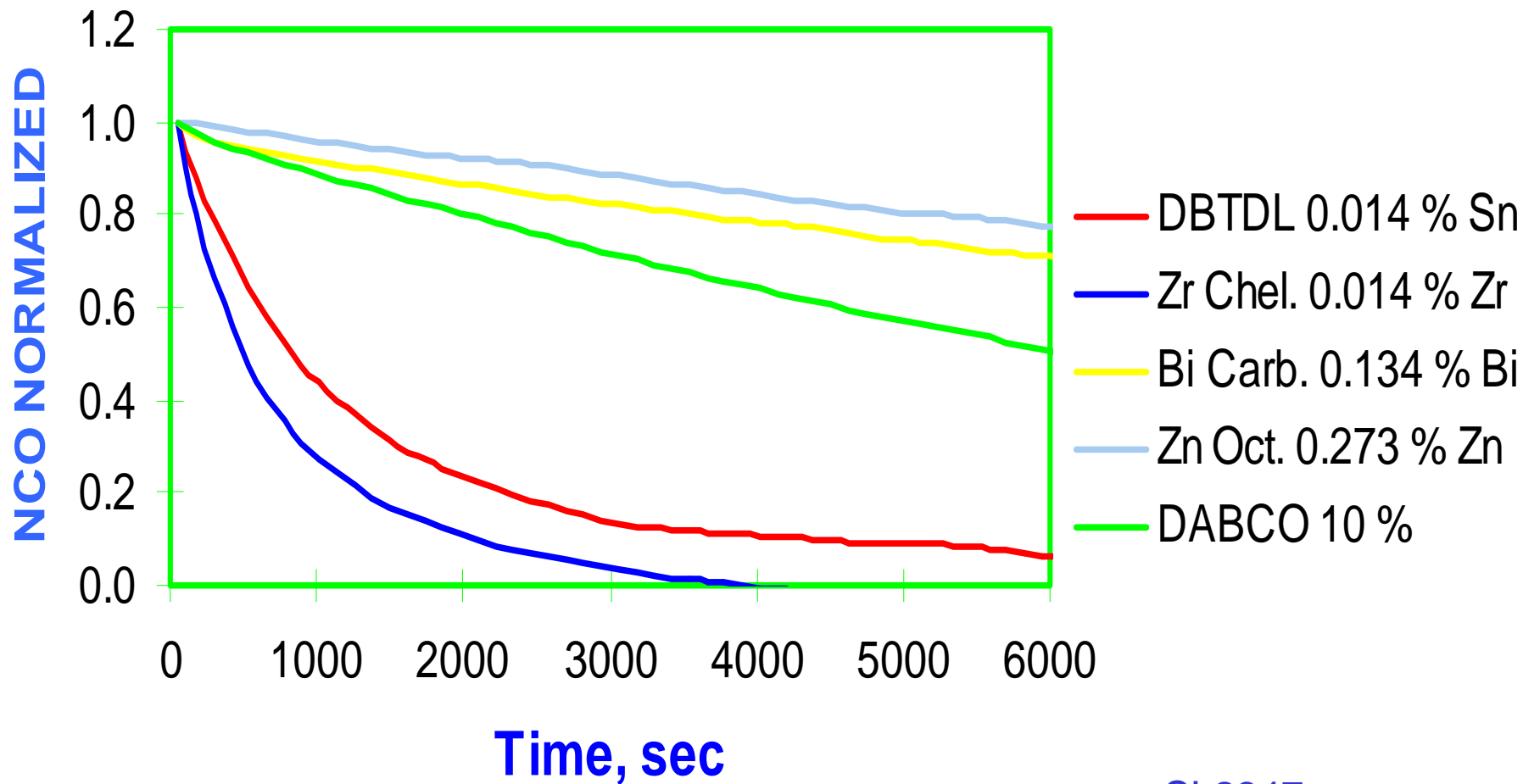
SL2345

HDI TRIMER / n-BUTANOL



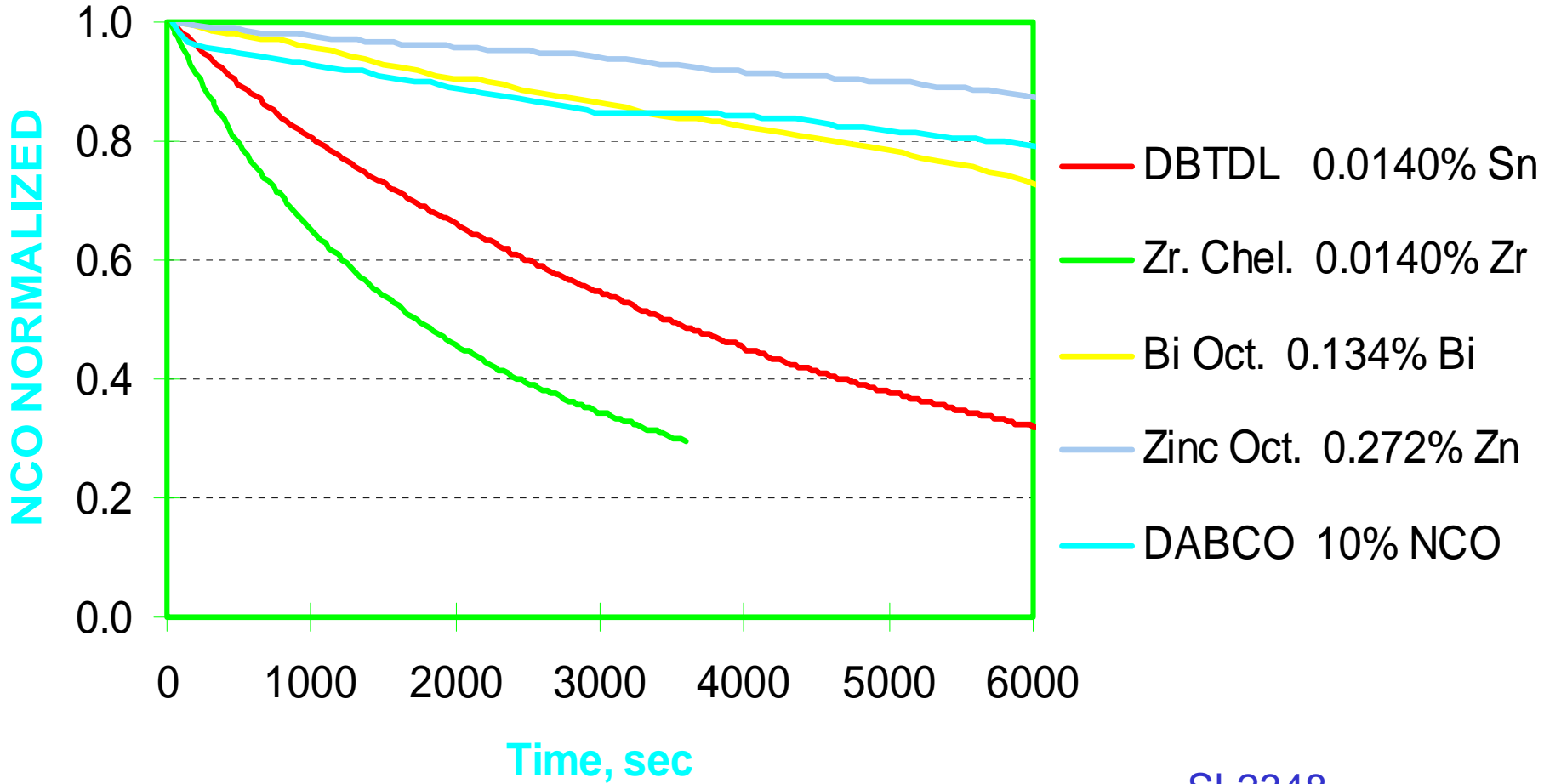
SL2346

HDI-TRIMER / ISOBUTANOL



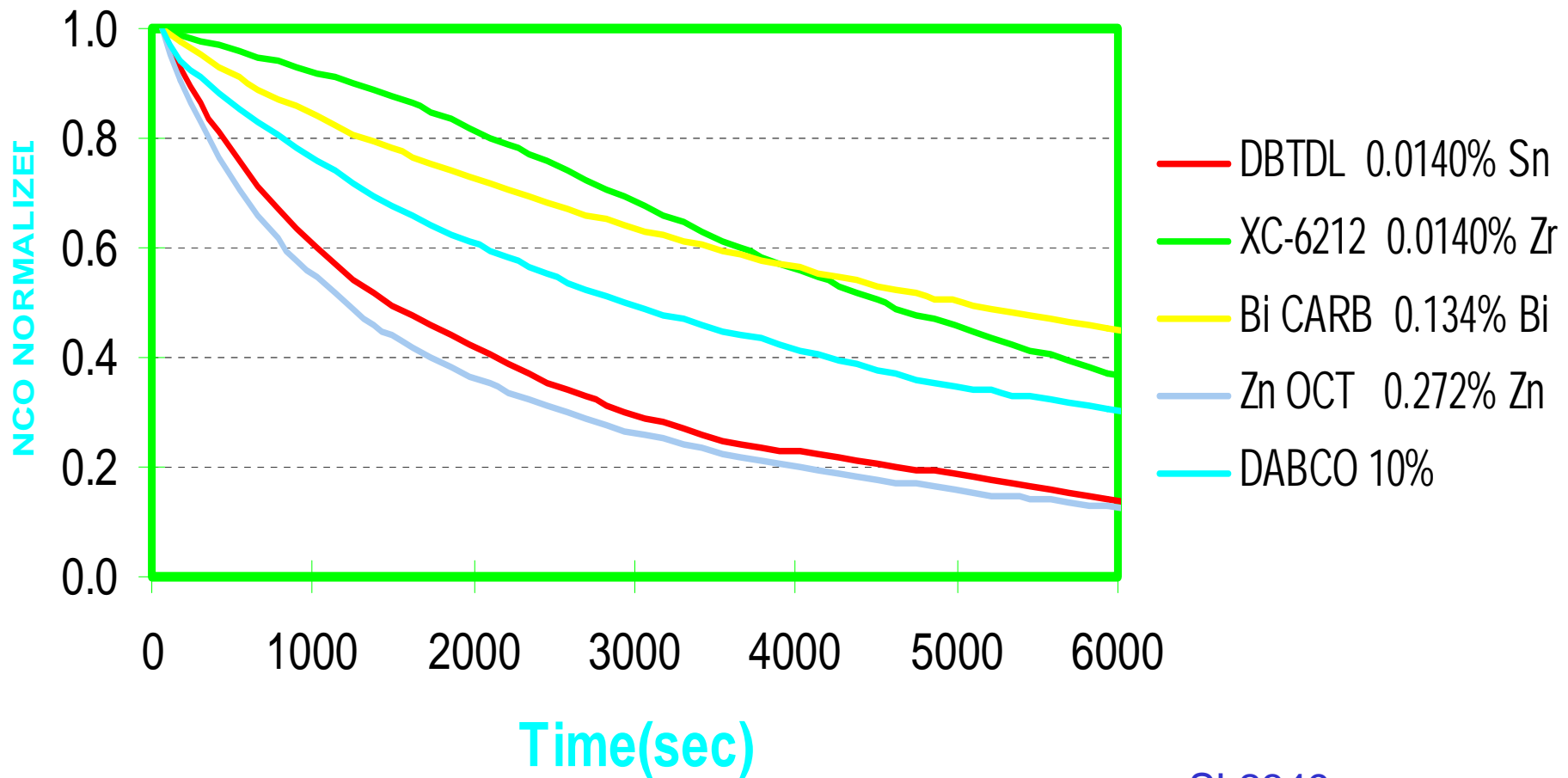
SL2347

HDI-TRIMER / 2-BUTANOL



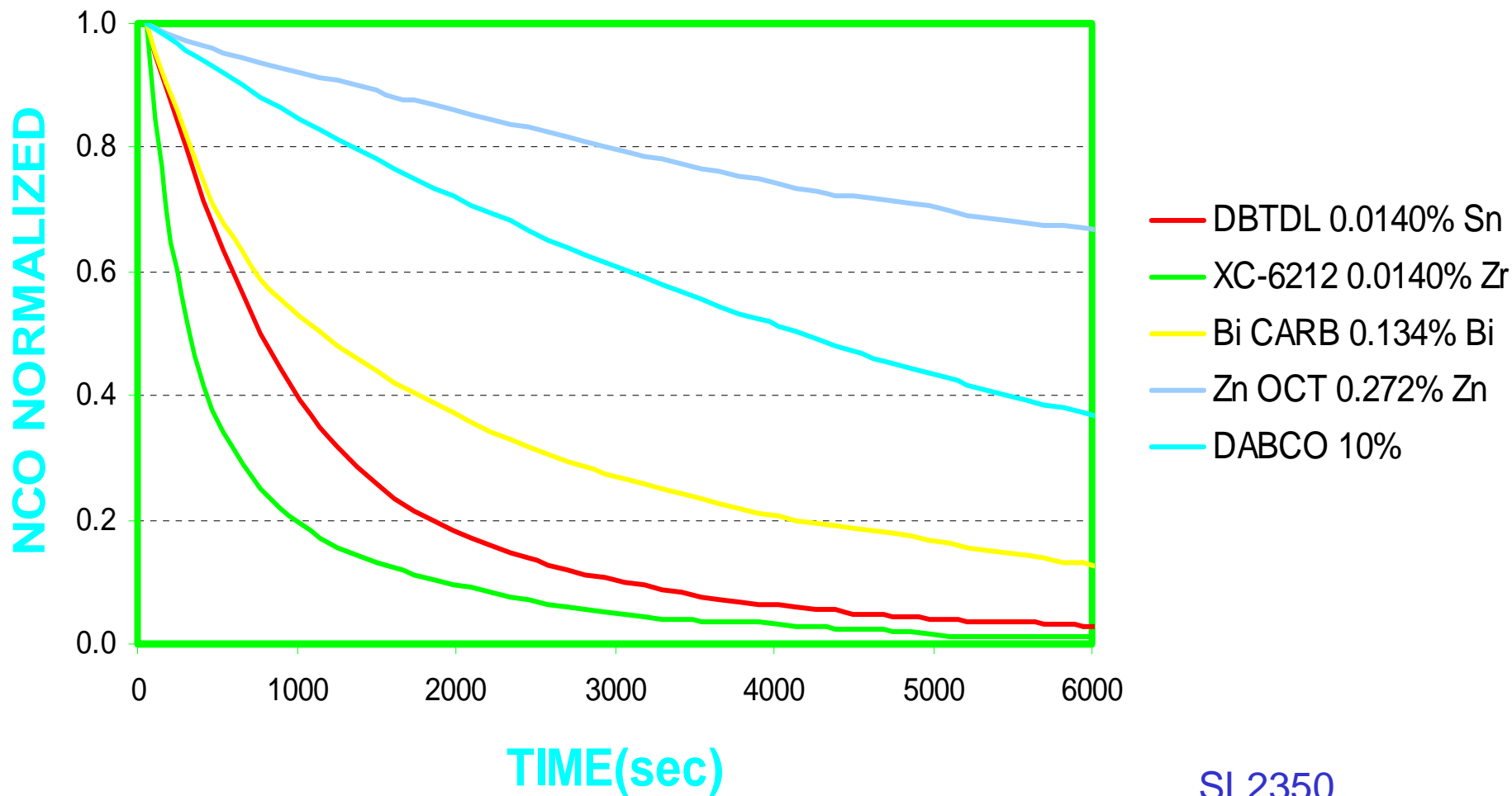
SL2348

HDI TRIMER / 2-BUTOXYETHANOL



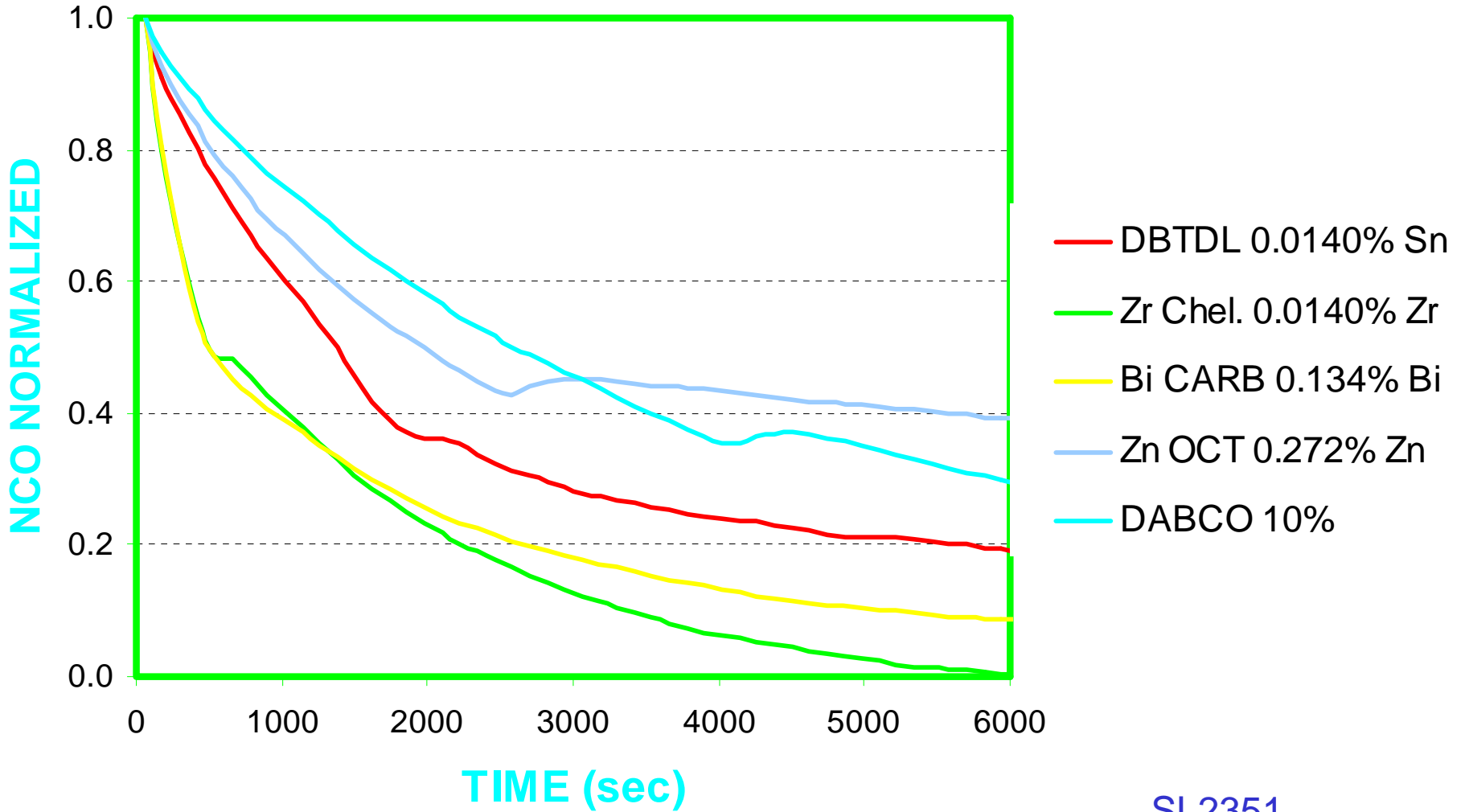
SL2349

HDI TRIMER / 2-HYDROXY ETHYL ESTER



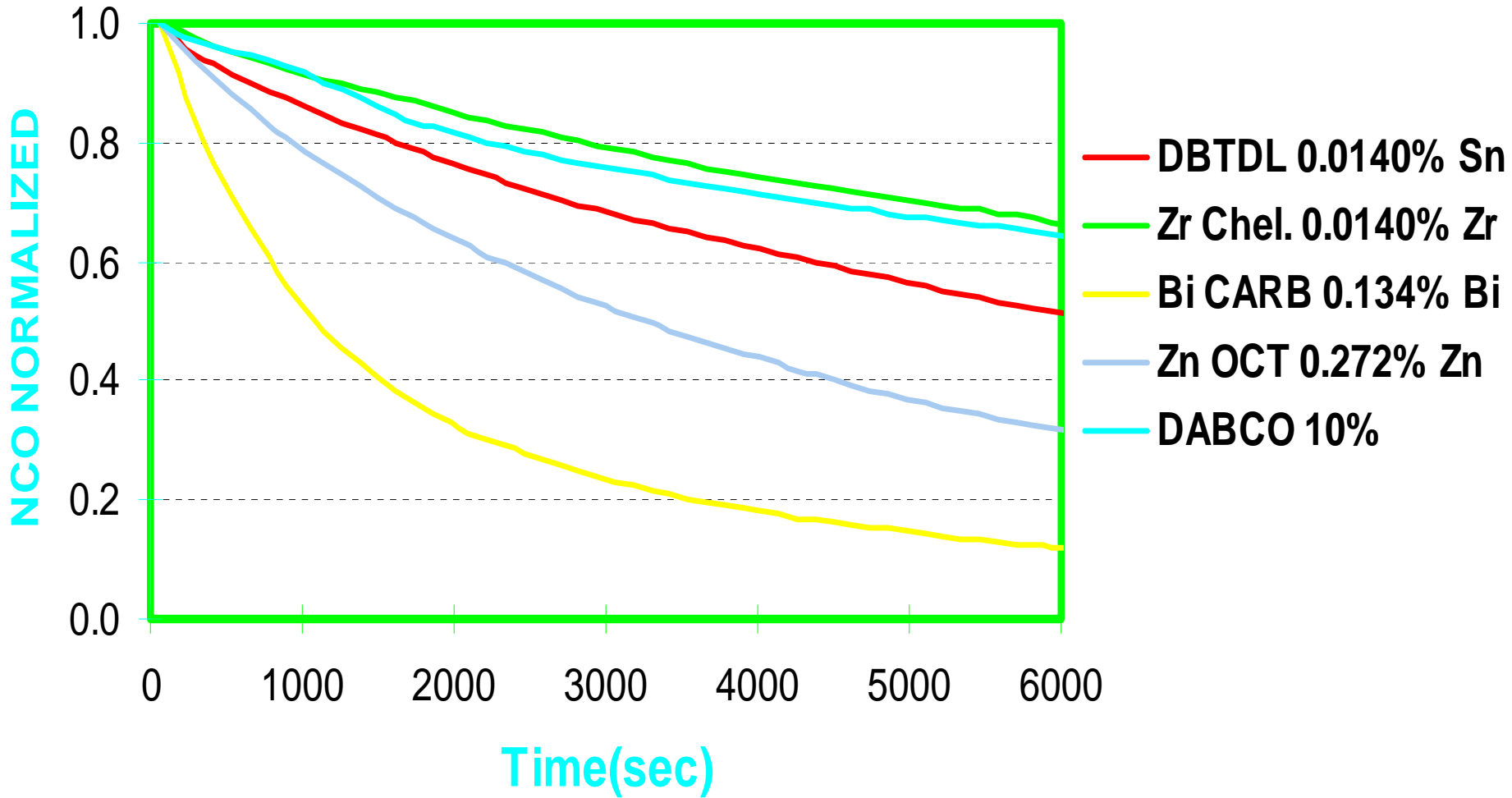
SL2350

HDI TRIMER / B-HYDROXY CARBAMATE



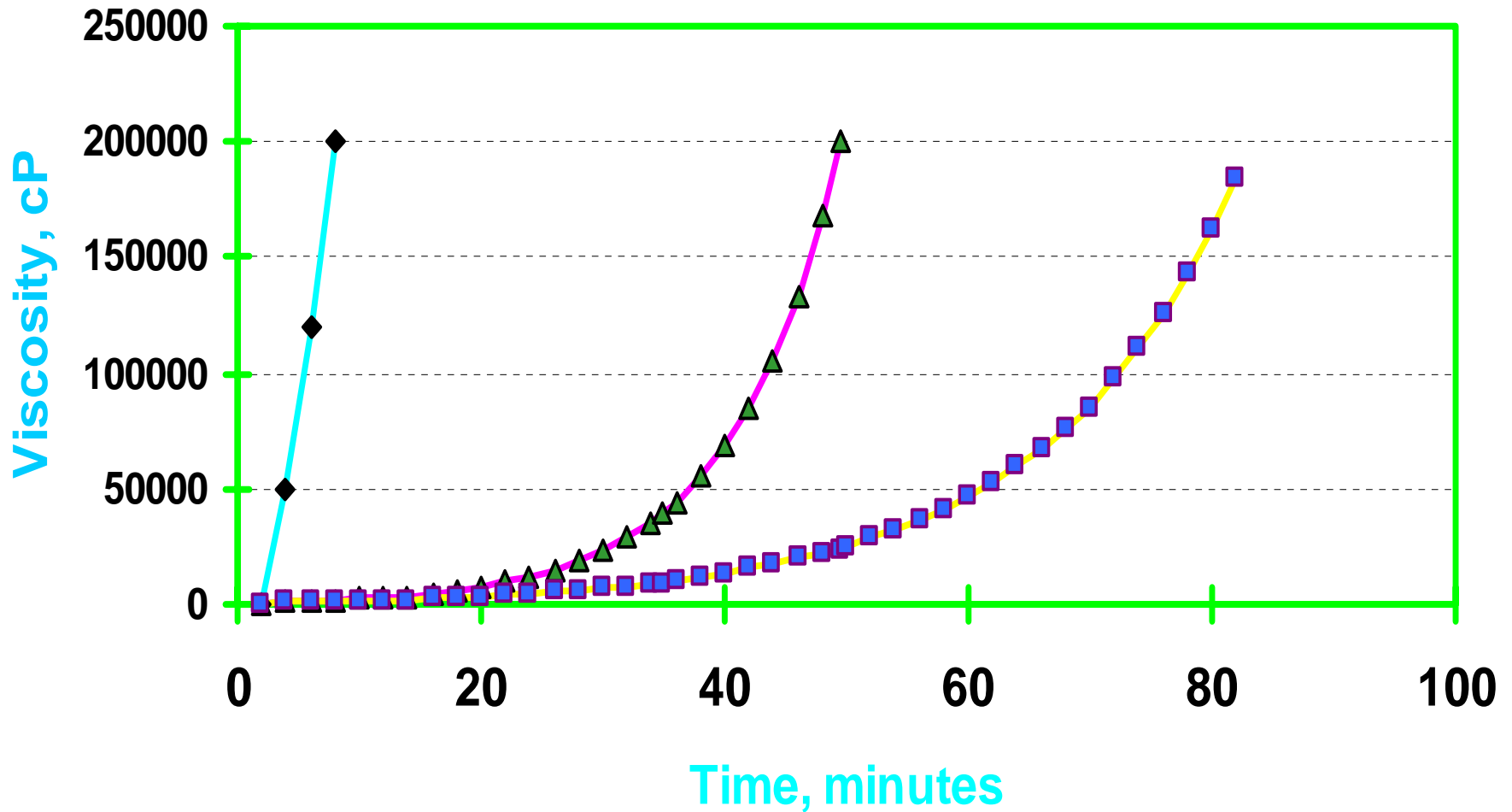
SL2351

HDI TRIMER / TPG-O-Me

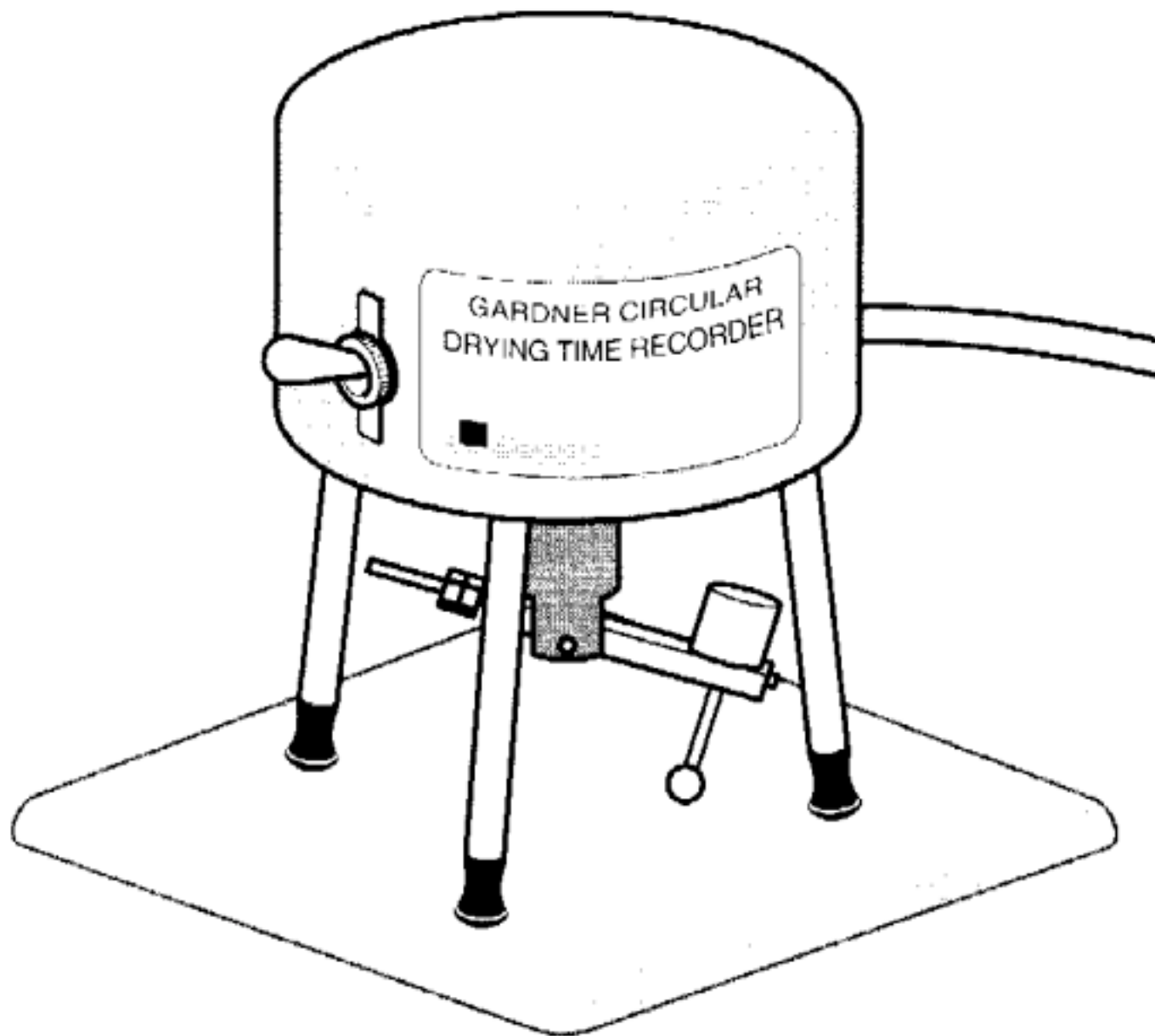


SL2352

Polyether MDI Elastomer Bi Oct. 1/5 mol WATER

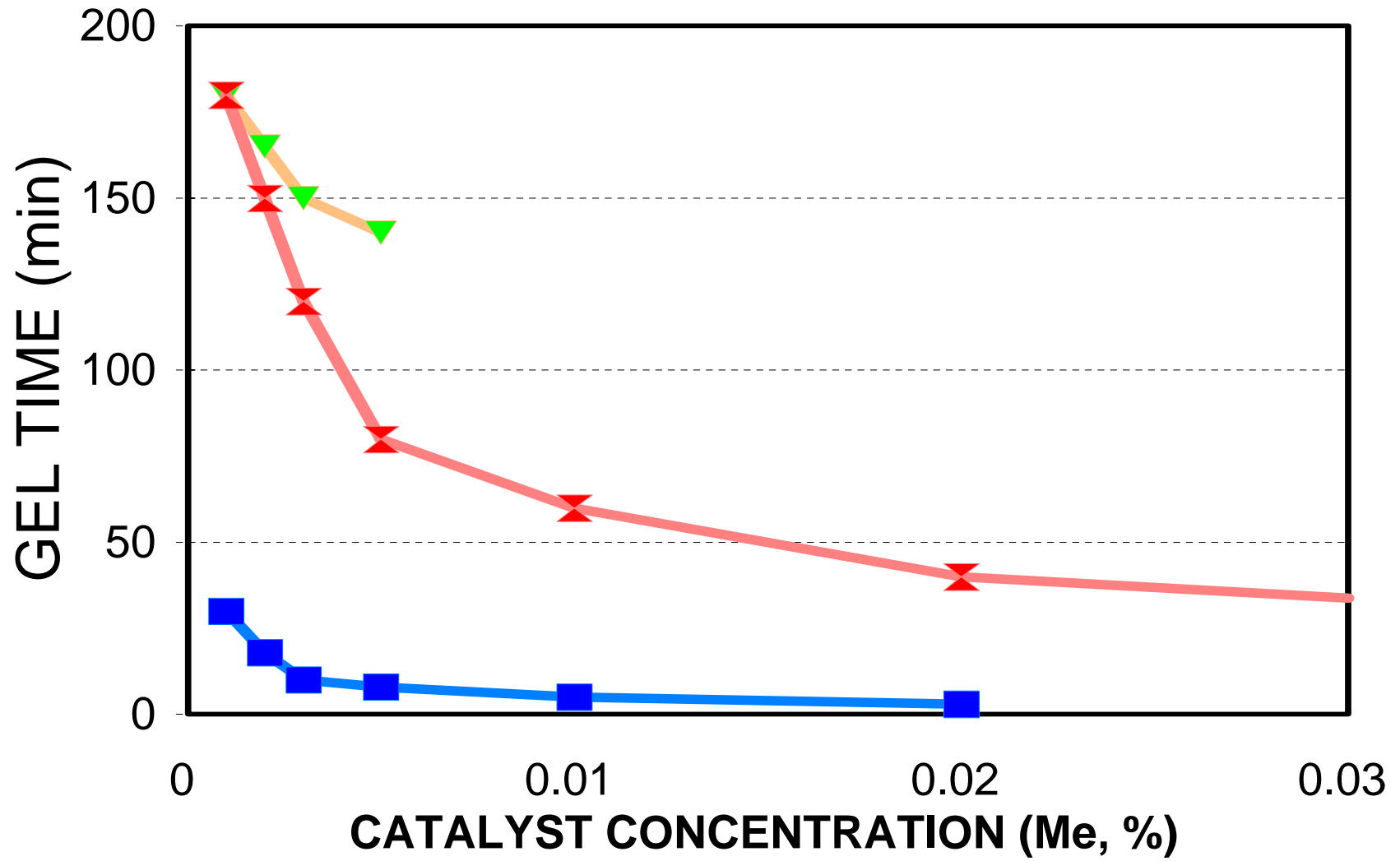


◆ Bi Oct. Initial ▲ Bi Oct. 2 days ■ Bi Oct. 7 days



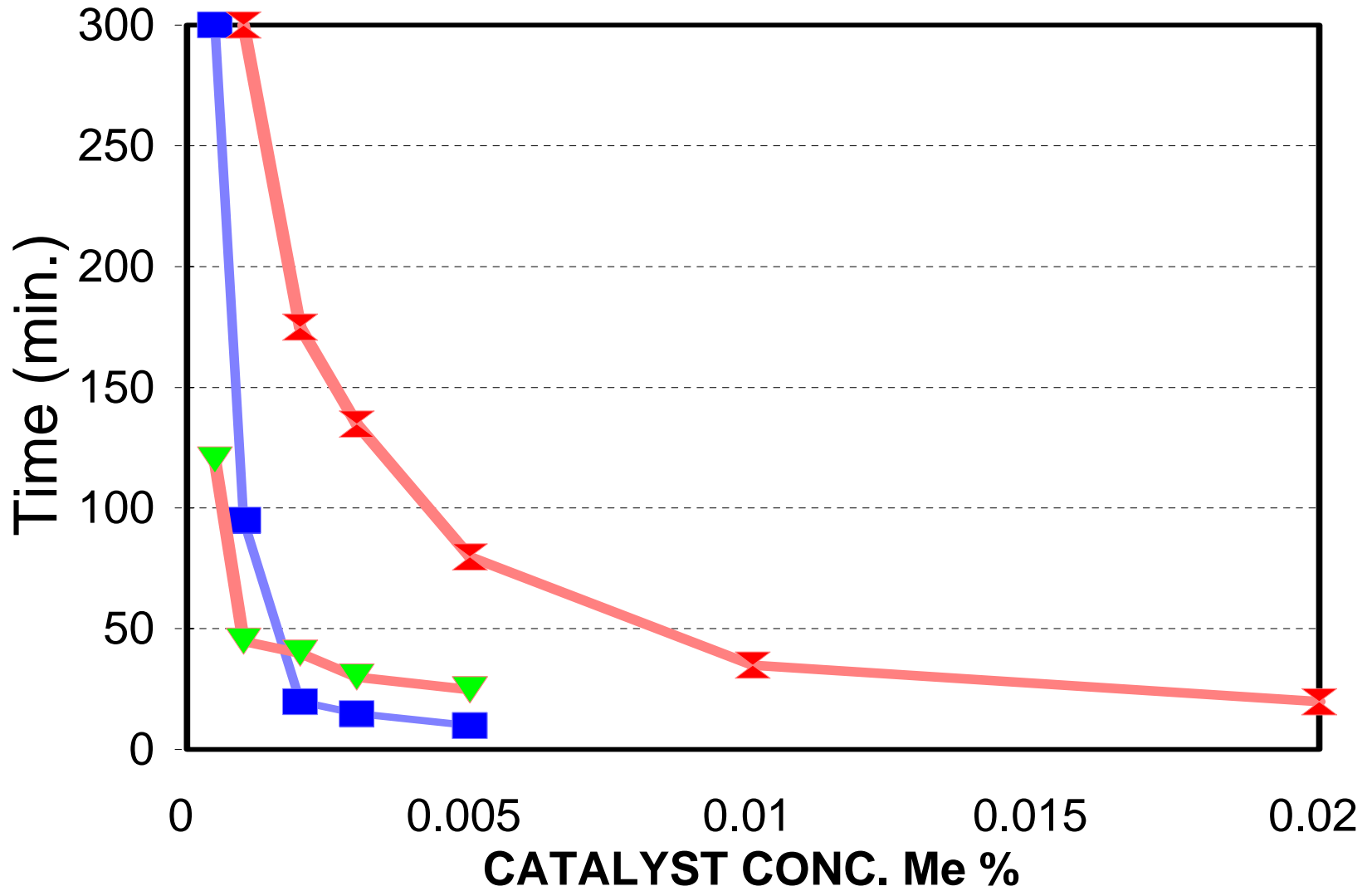
GEL TIME

ACRYLIC/HDI-TIMER



■ Zr B ▼ Zr A × DBTDL

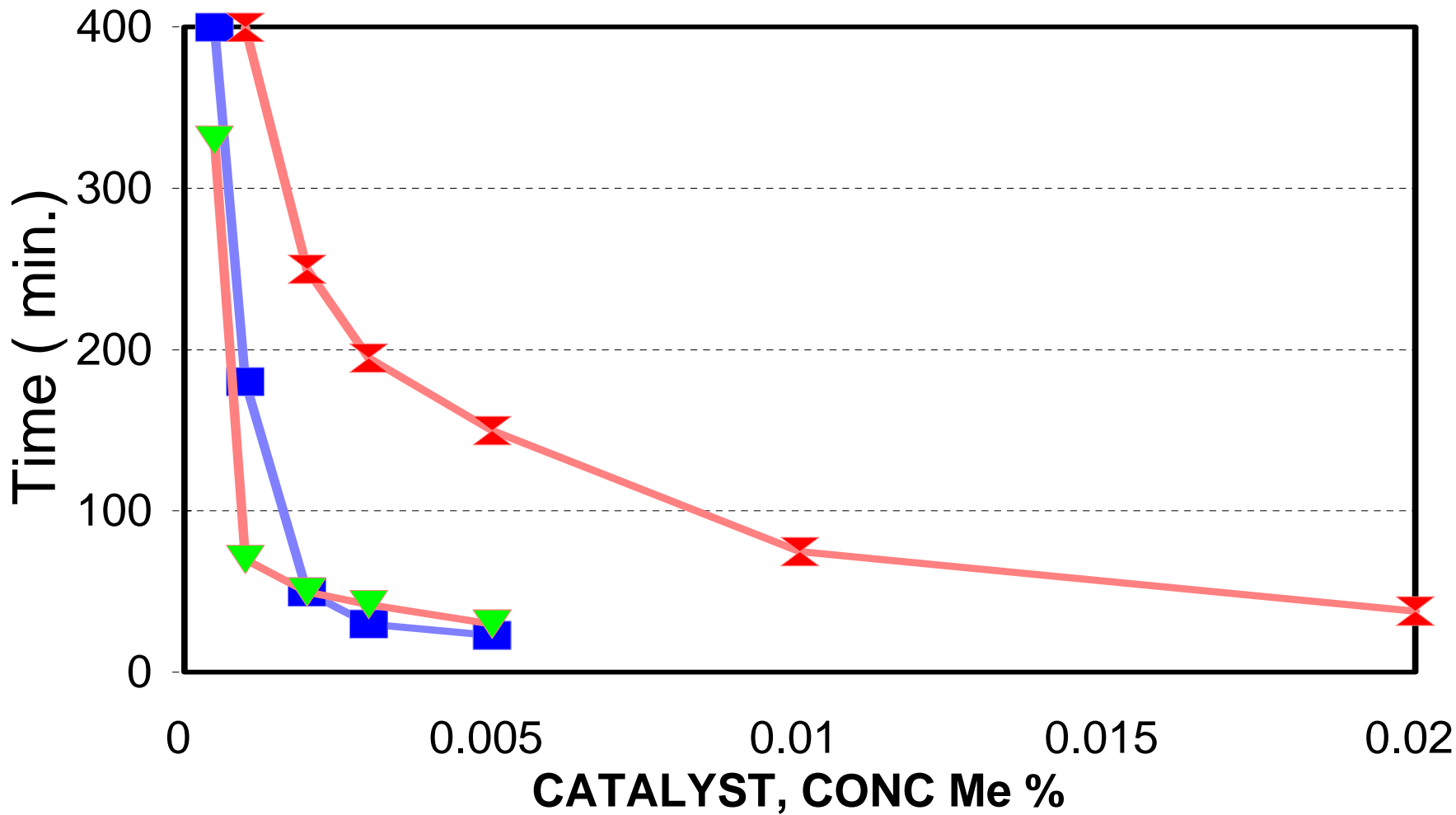
Tack Free time Acrylic HDI-Trimer



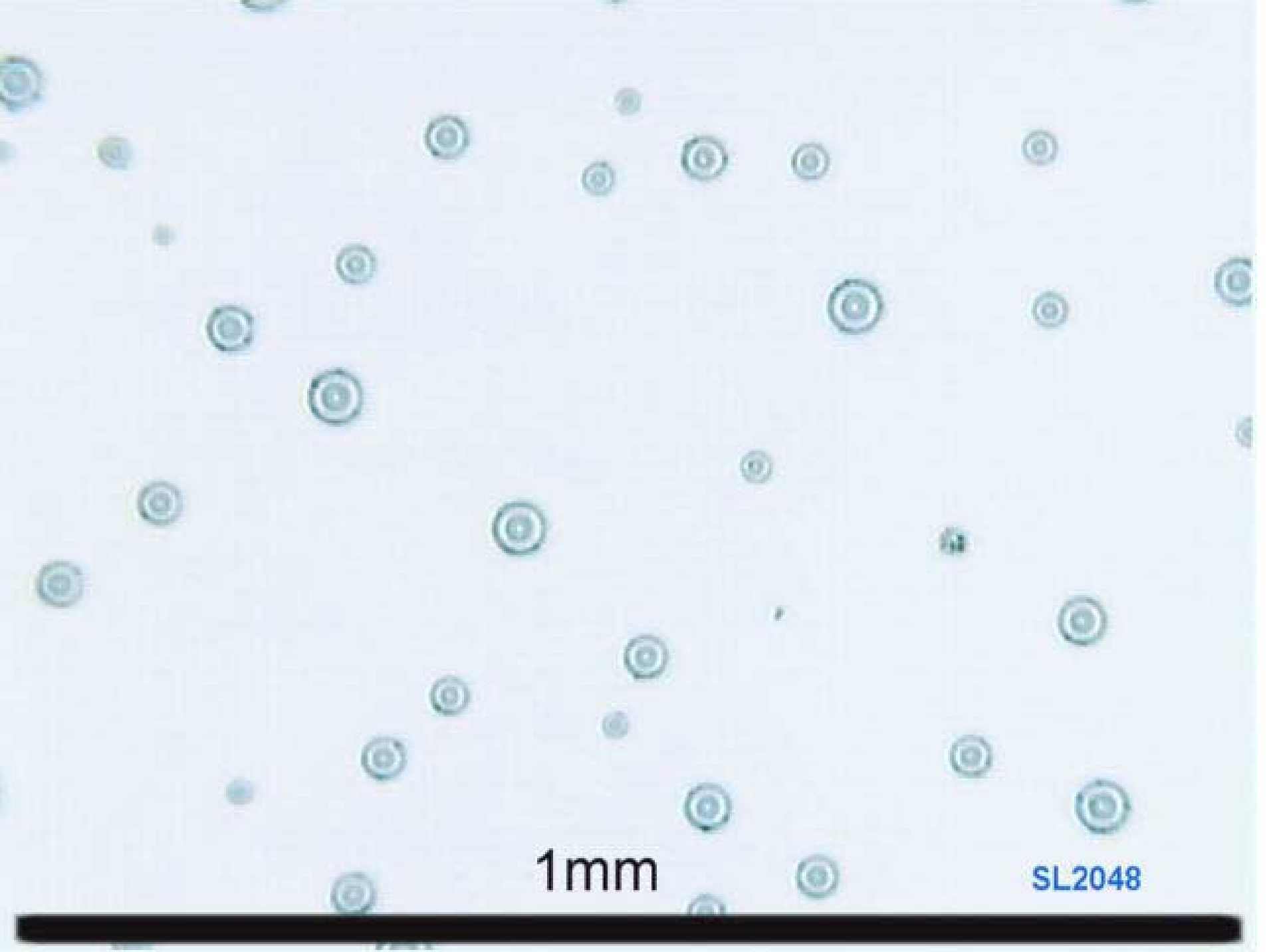
■ Zr B ▼ Zr A × DBTDL

DRY THROUGH TIME

ACRYLIC/HDI-TRIMER, 30 μ , RT, 66 % RH



■ Zr B ▼ Zr A × DBTDL



1mm

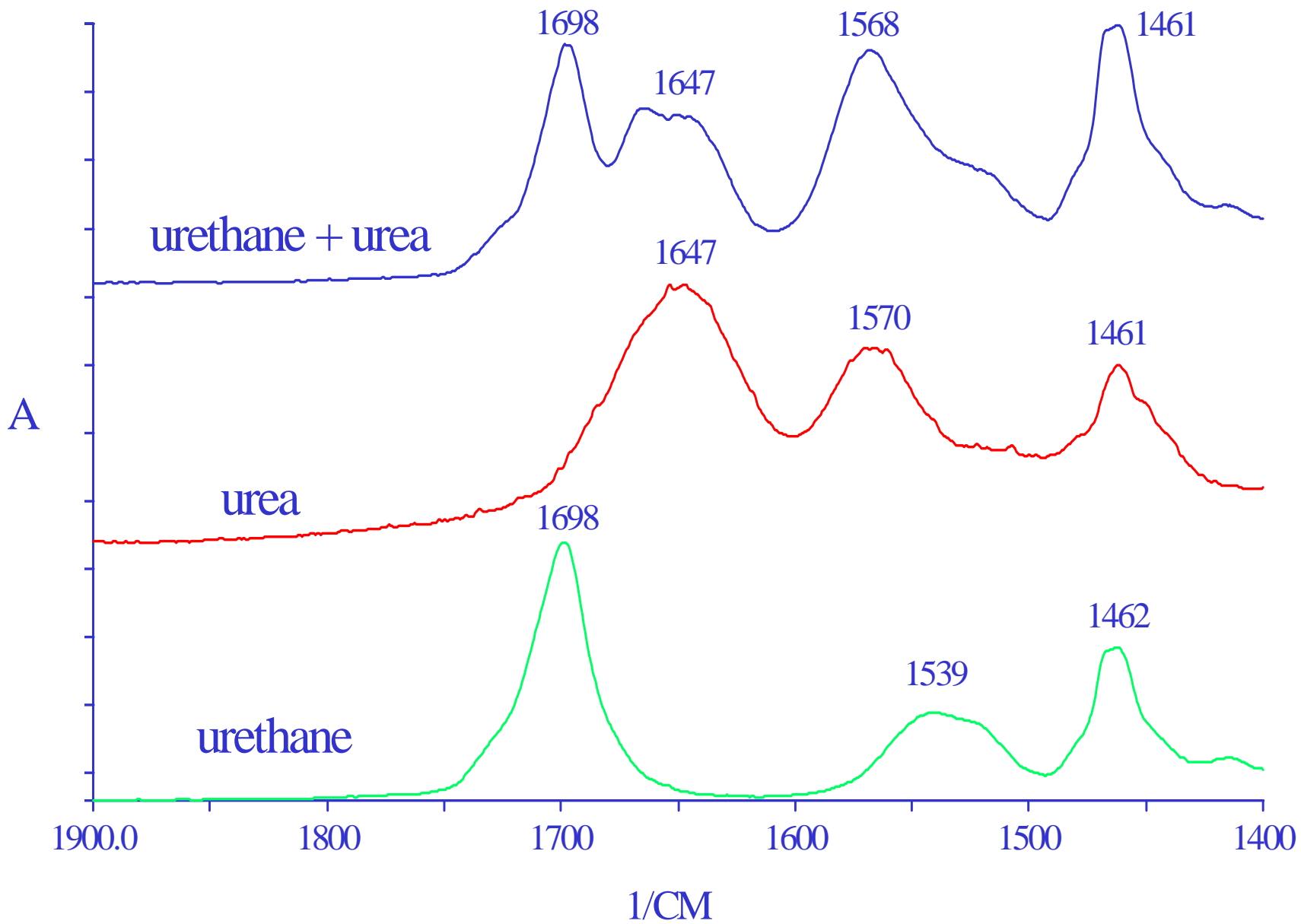
SL2048

**HDT-LV ISOCYANATE
WATER (2%) 0.0045 % Me**



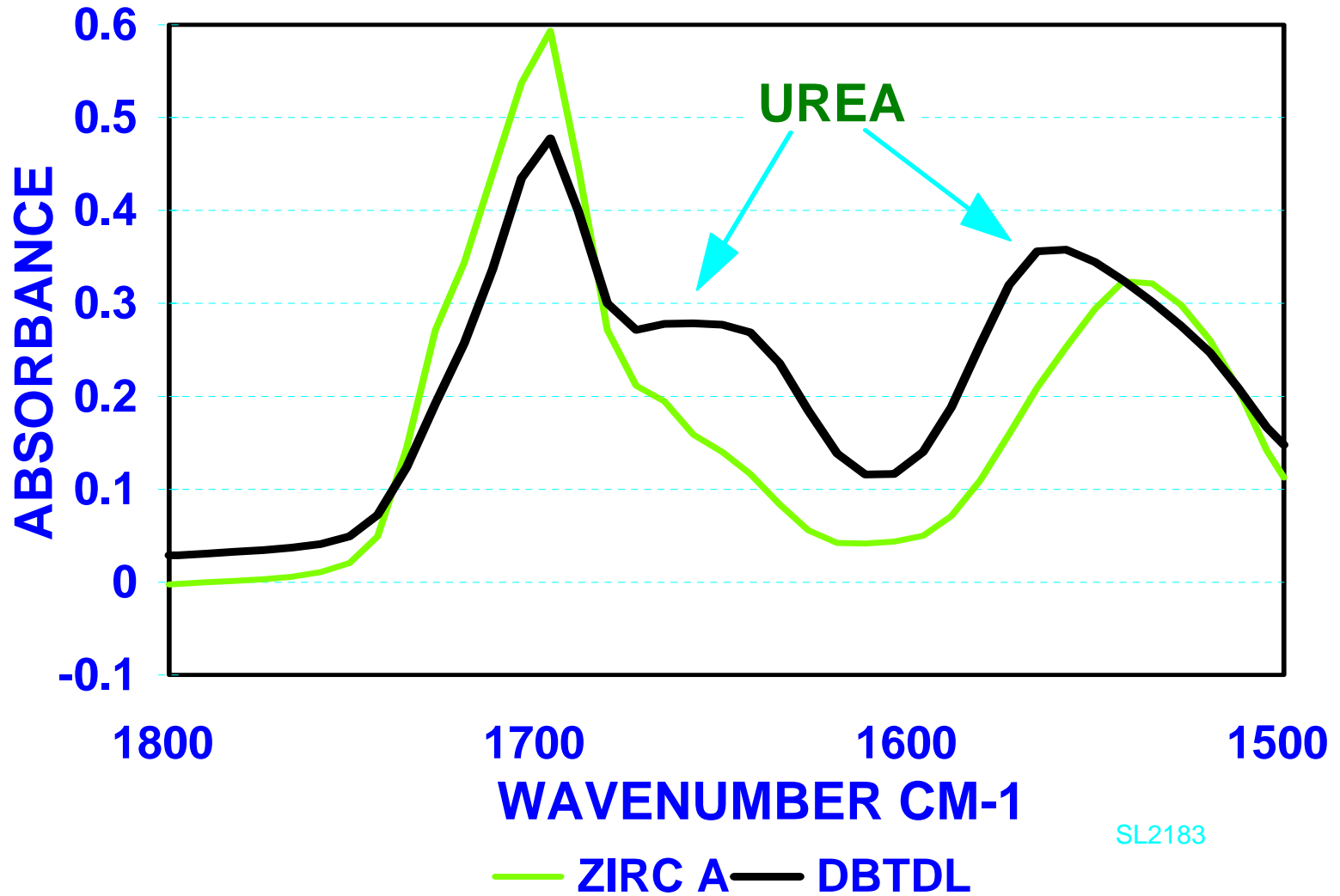
K-KAT XC-4205

DBTDL

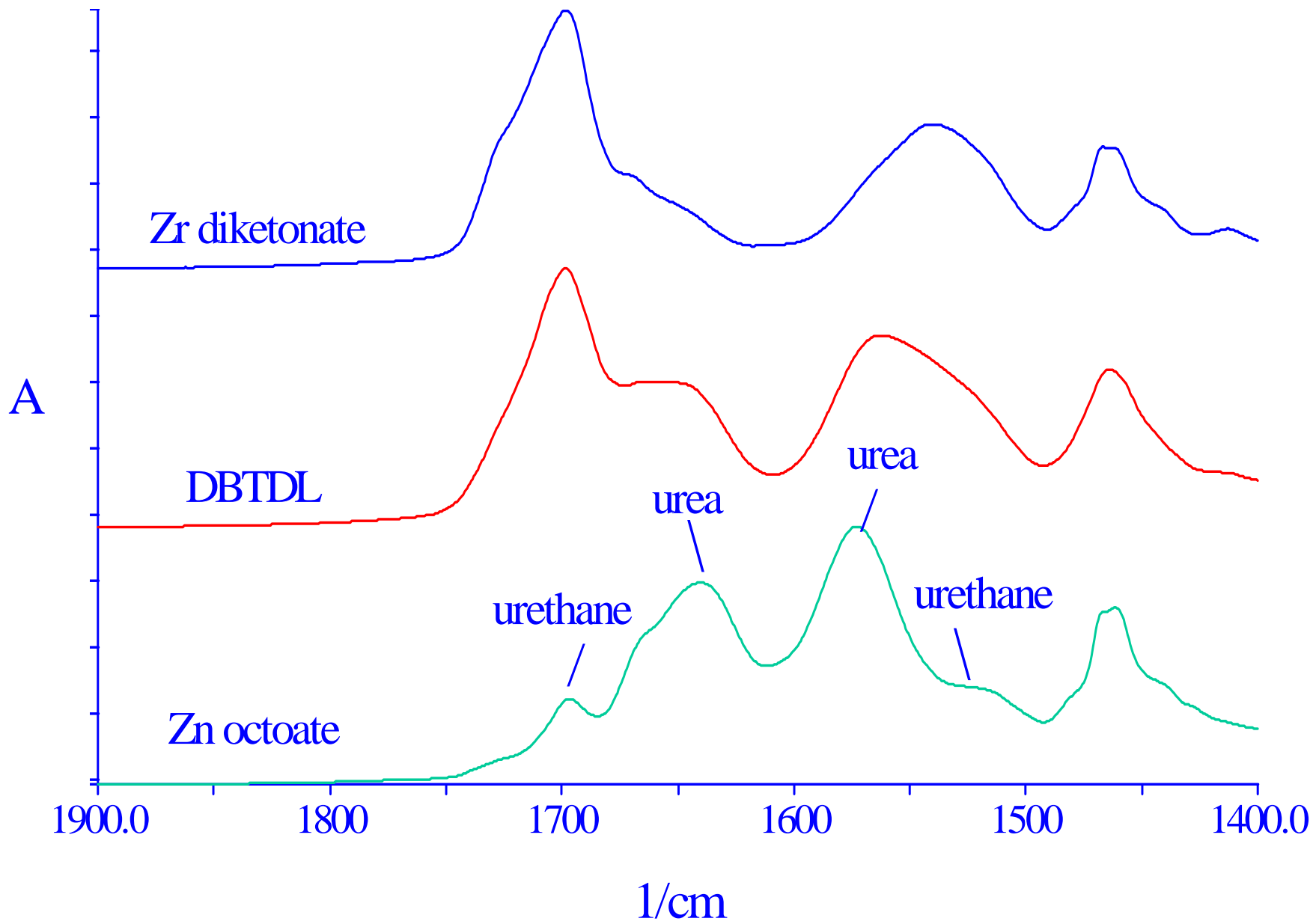


SELECTIVITY OF CATALYSIS

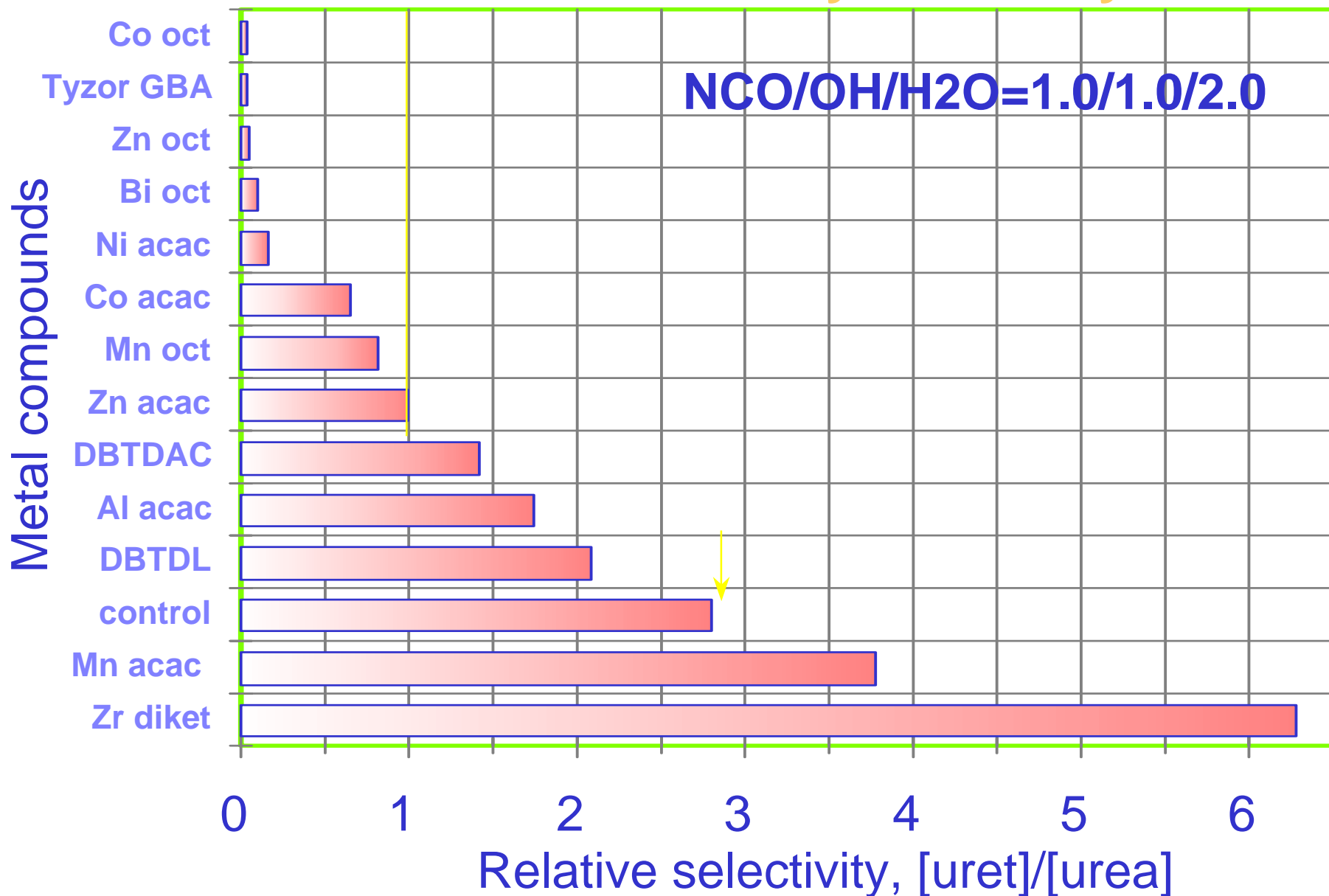
DBTDL & Zr CHELATE



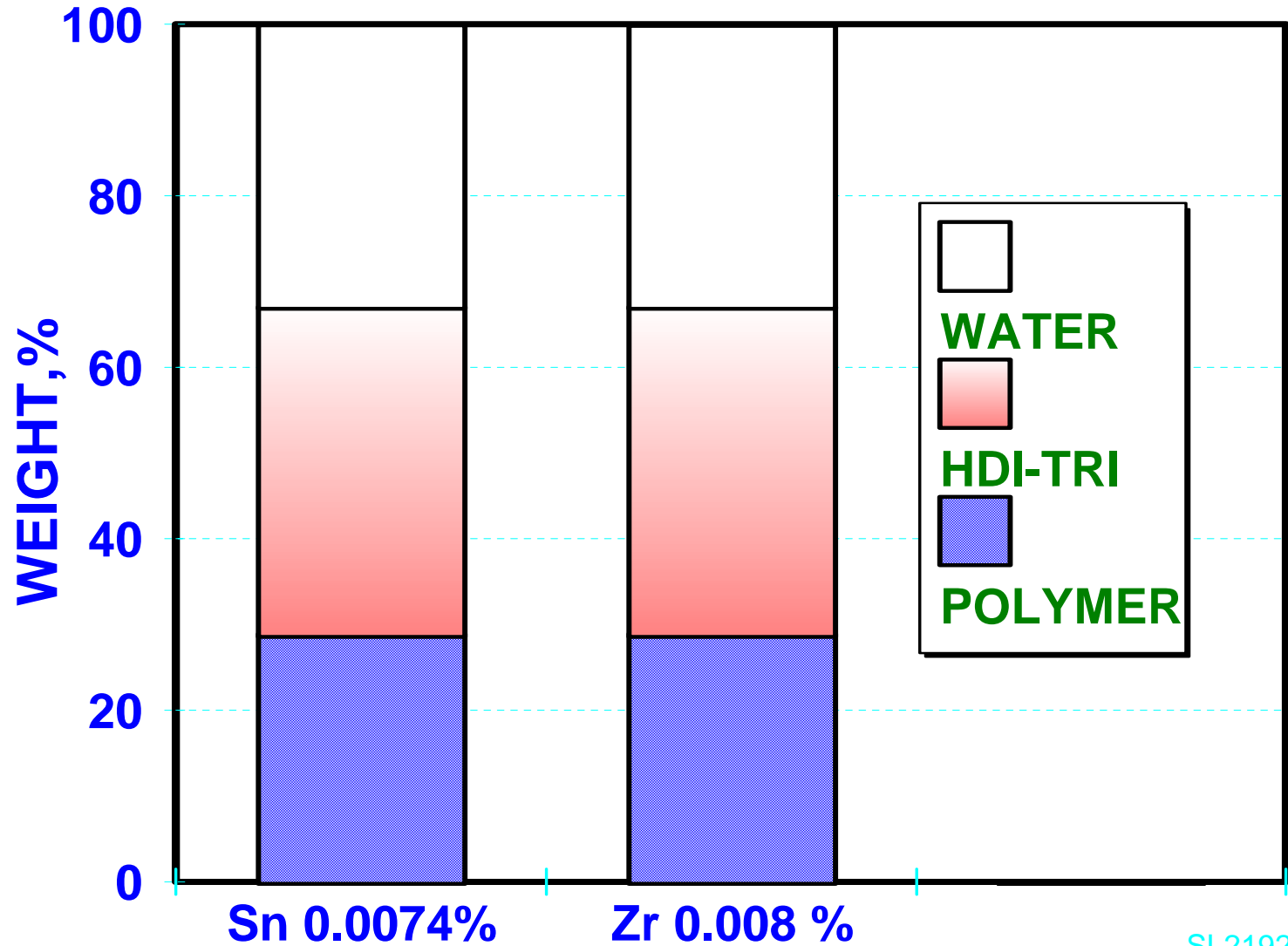
SL2183



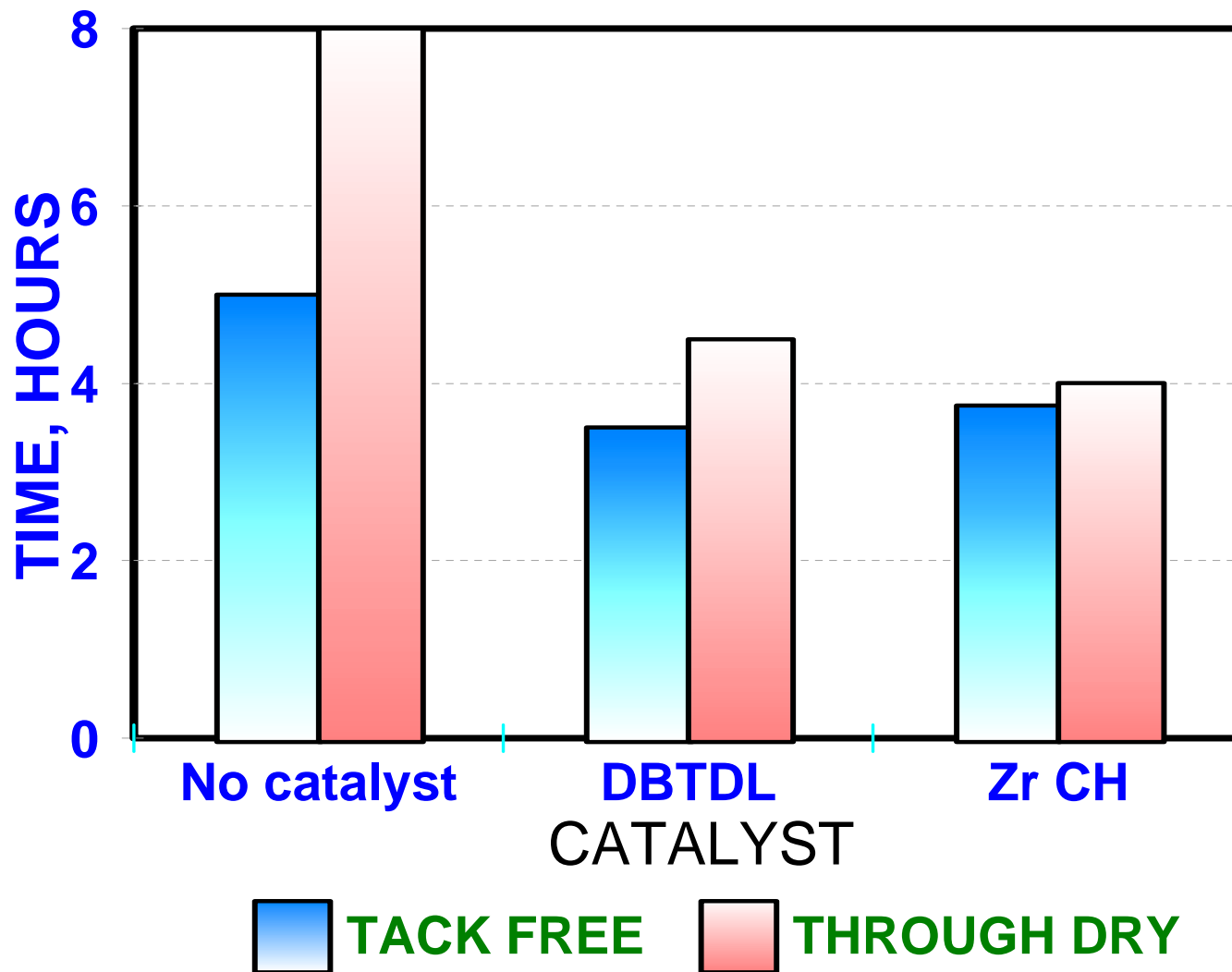
Relative Selectivity vs. Catalysts



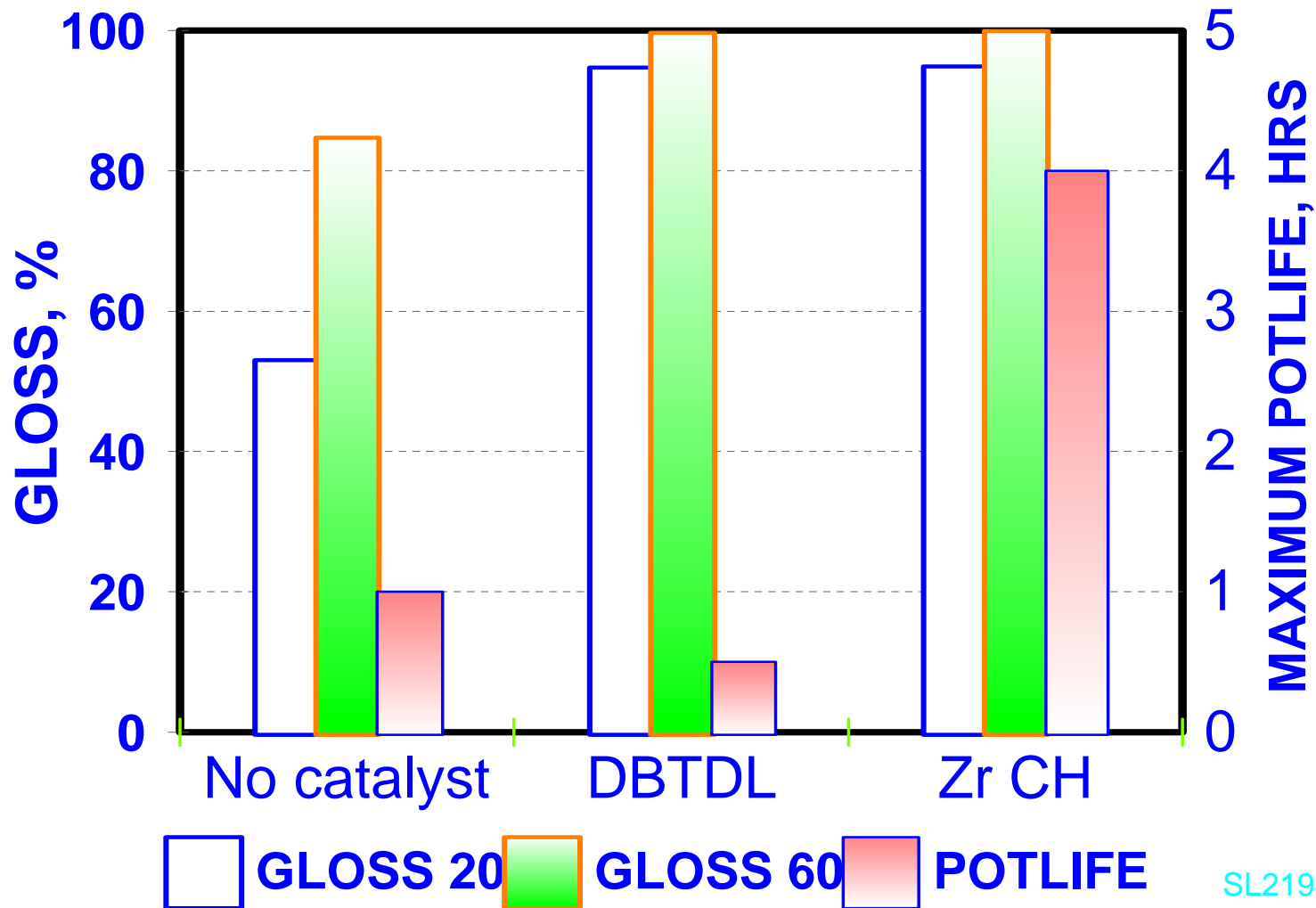
WATERBORNE TWO COMPONENT



WATERBORNE TWO COMPONENT



WATERBORNE TWO COMPONENT CATALYST SELECTION



WATERBORNE TWO COMPONENT

XC-6212

XC-6212

DBTDL



A100 XC6212 0H RT 496-10

0 HOUR



A107 XC6212 RT 496-10

4 HOURS



A111 DBTDL 0.5H RT 496-10

1/2 HOUR

WATERBORNE TWO COMPONENT

XC-6212

XC-6212

XC-6212



A100 XC6212 OH RT 496-10

50 % RH

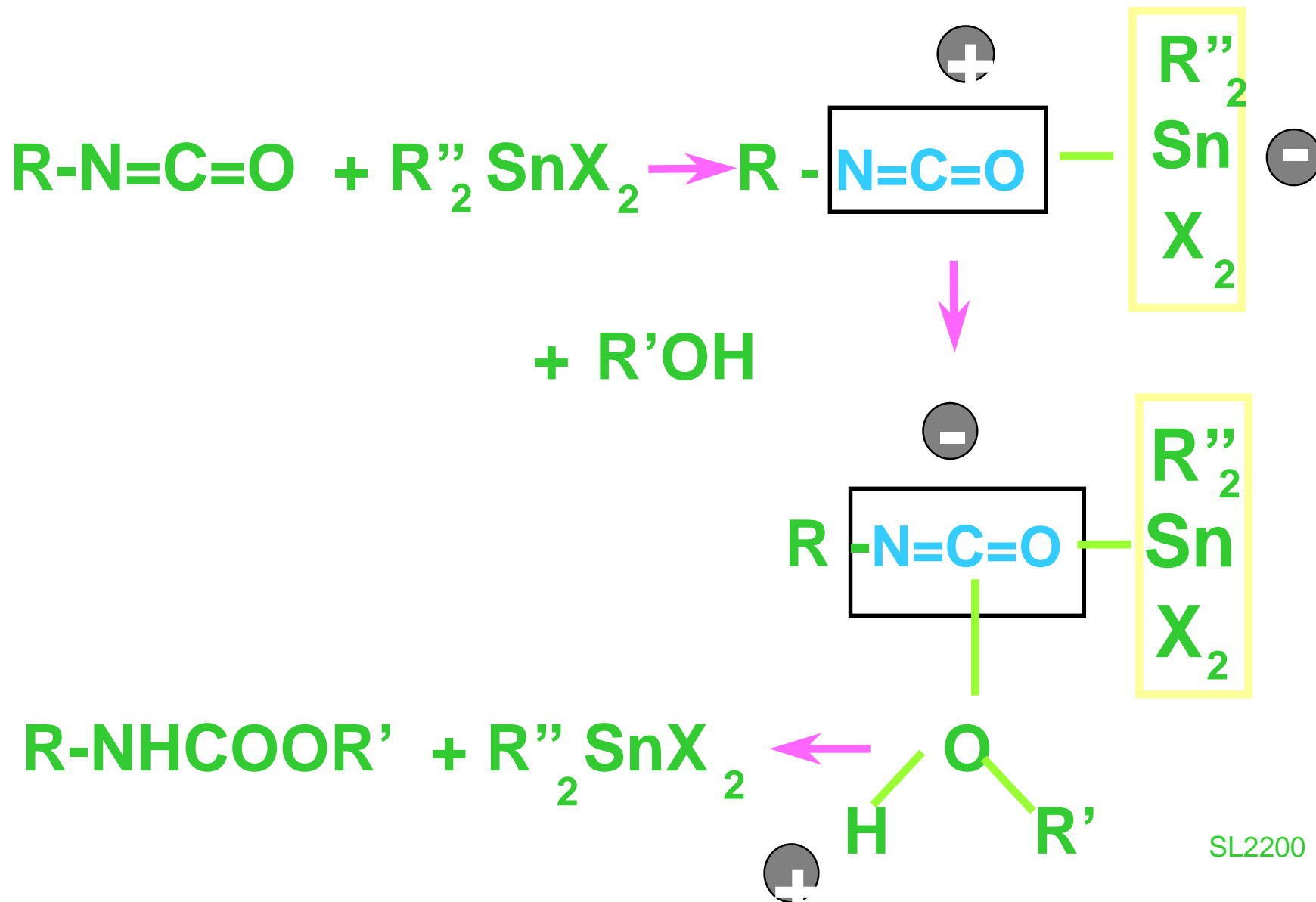
A108 XC6212 OH 70RT 496-10

70 % RH

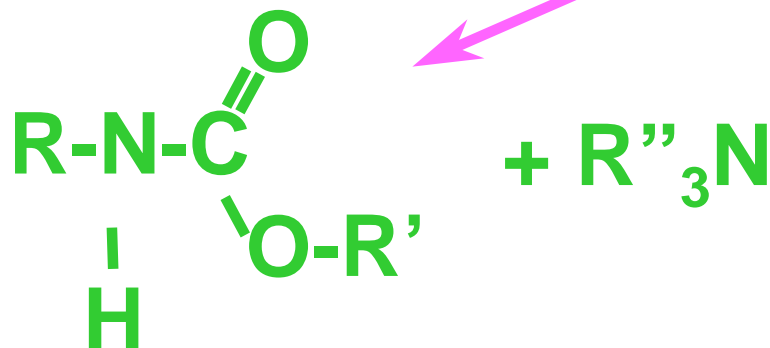
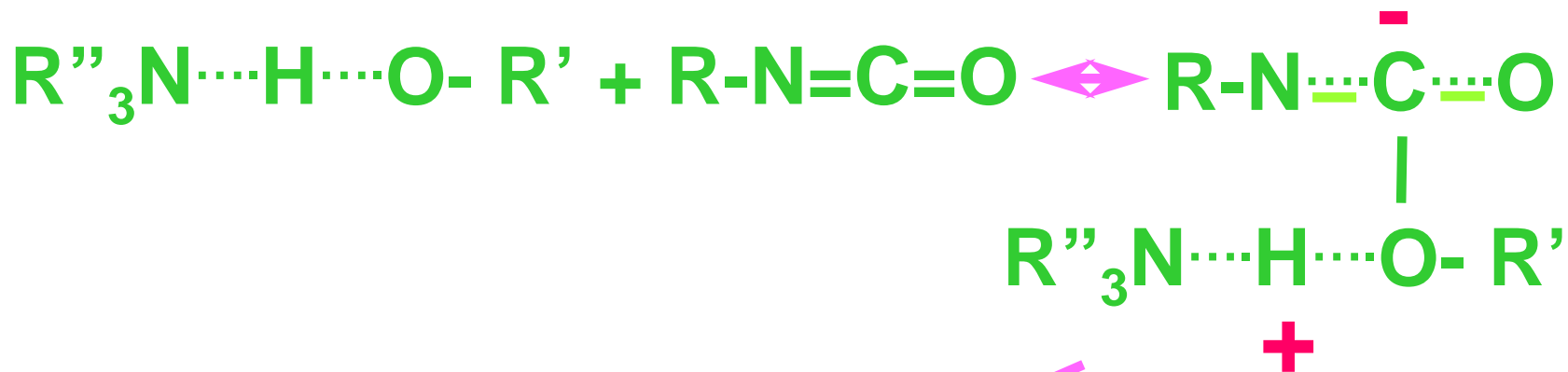
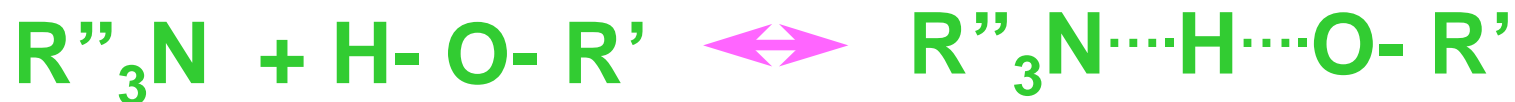
A100 XC6212 OH 90RT 496-10

90 % RH

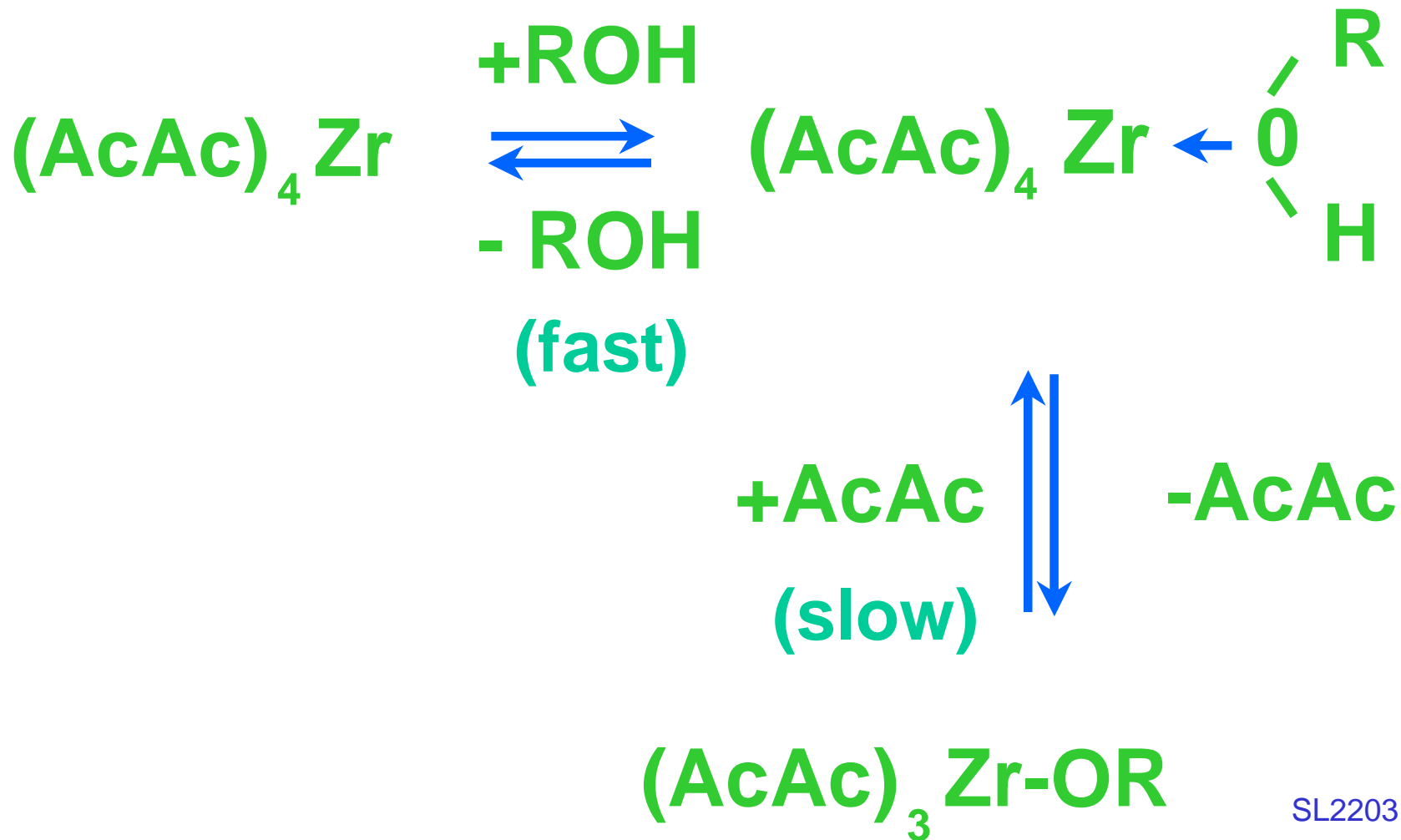
LEWIS ACID CATALYSIS



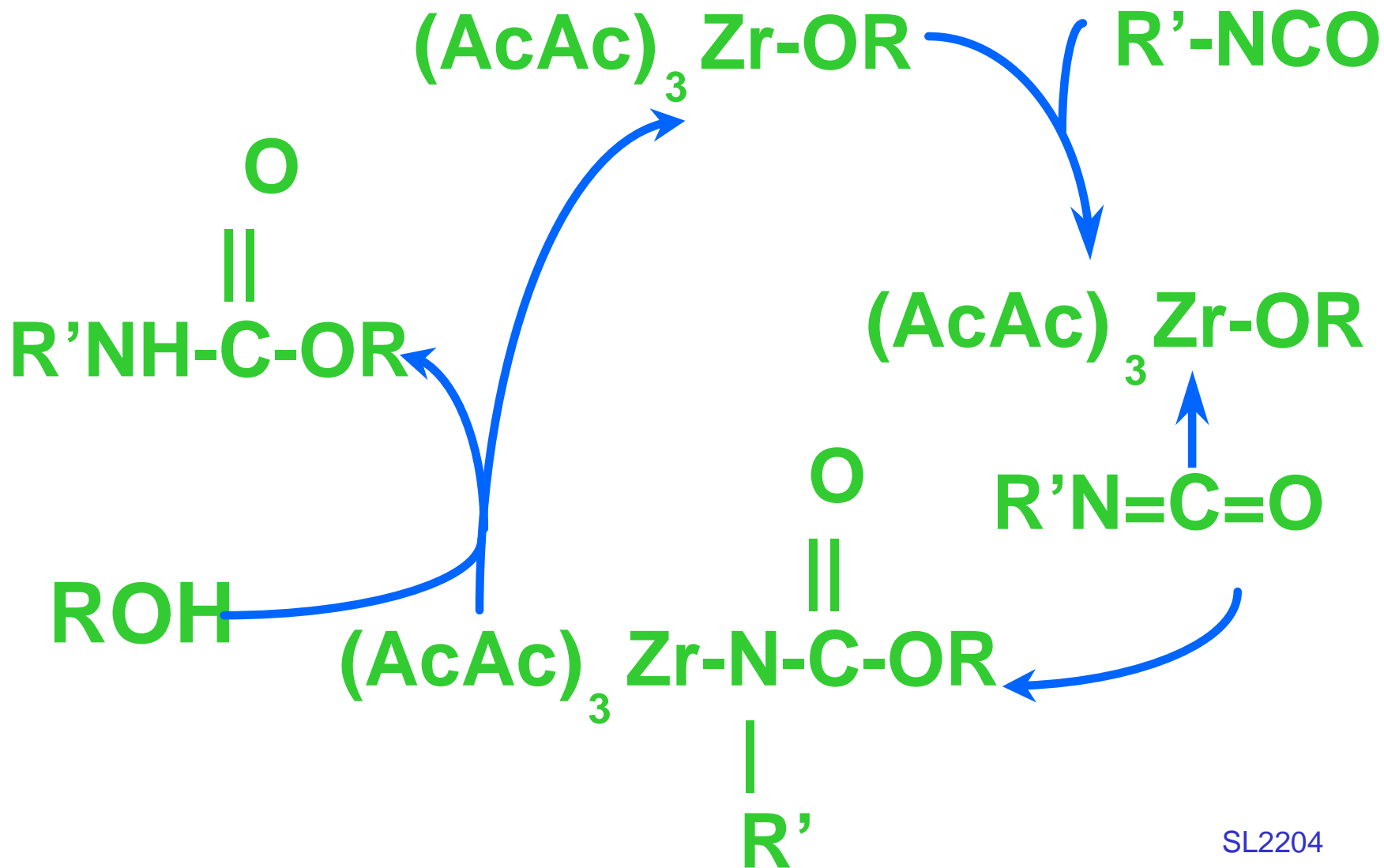
AMINE CATALYSIS



ZIRCONIUM CHELATE CATALYSIS



ZIRCONIUM CHELATE CATALYSIS

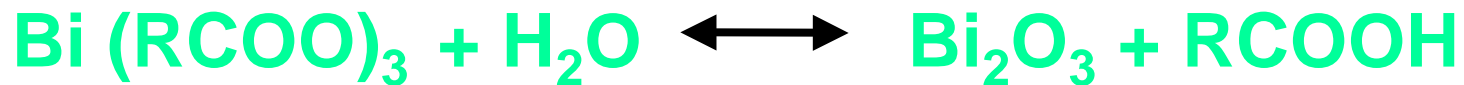


HYDROLYSIS OF Zr CHELATE

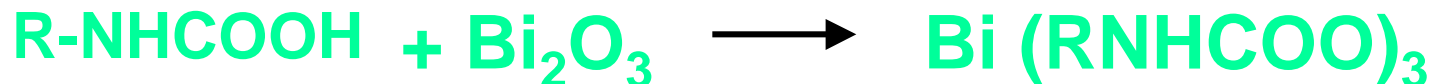
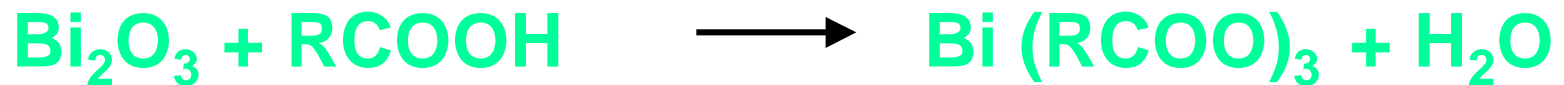


DELAYED ACTION OF BI CARBOXYLATE

DEACTIVATION



ACTIVATION



SUMMARY

ORGANO TIN FREE COATINGS POSSIBLE

CHOICE OF CATALYST DEPENDS ON APPLICATION

Zr CHELATE ACTIVATES HYDROXYL

Zr CHELATE CATALYSTS SELECTIVE FOR OH

HIGH REACTION RATES POSSIBLE

RELATIVE REACTIVITY OF HYDROXYLS DIFFERENT

CATALYSIS OF WATERBORNE COATINGS WITH Zr

ACKNOWLEDGEMENT

TECHNICAL SERVICE DEPARTMENT

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