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# **A Selective Catalyst for 2K WB Polyurethane Coatings**

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Picci**

**King Industries, Inc.**



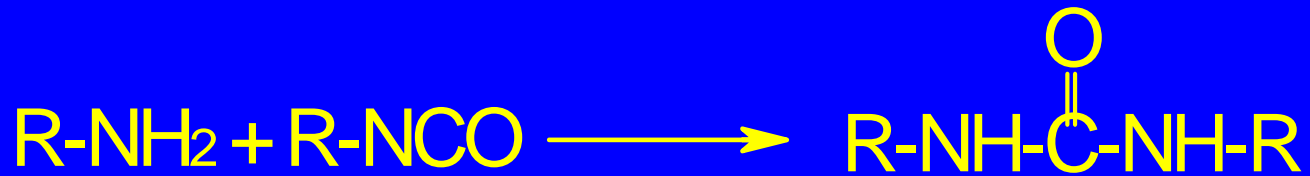
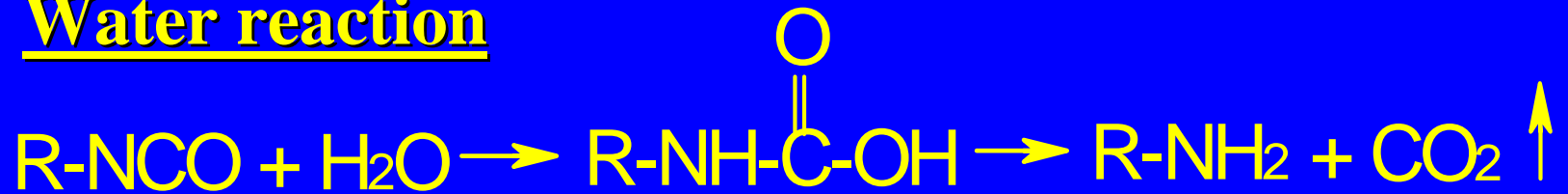
# Outline

- **Introduction**
- **Objectives**
- **Experimental Approaches**
- **Results and Discussions**
- **Conclusions**

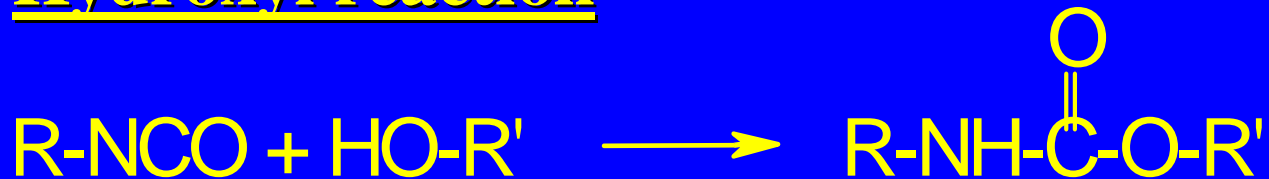
## Driving Force for 2K WB PU

- **High Performance**
- **Low/no VOC**

### Water reaction



### Hydroxyl reaction



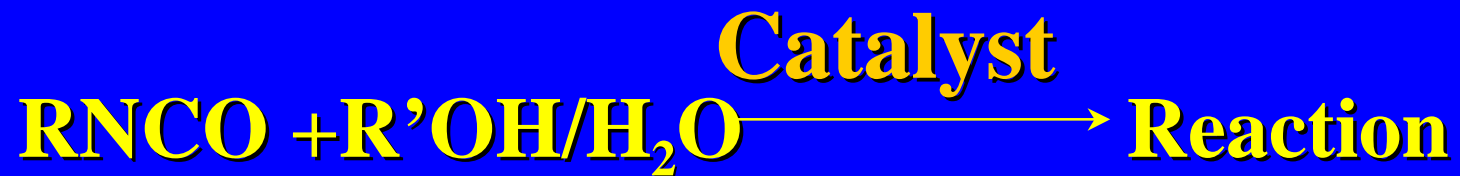
## Problems of NCO/H<sub>2</sub>O

- **Gassing/foaming**
- **Loss of gloss**
- **Reduced pot life**
- **High NCO demand**

**Physical Approaches:      end users%**

- **2K Plural Spray Gun                      50 %**
- **Thin Film                                      20 %**
- **Low Humidity level                      20 %**
- **Require all three                              2 %**

## A novel chemical approach:



**Control NCO/H<sub>2</sub>O reaction  
with a selective catalyst**

## Previous Studies on Selectivity

- **DBTDL & DBTDCh in diff. solvents**
- **DBTDL, DABCO & Hg on NCO/H<sub>2</sub>O**
- **Diff. in amine catalyzed NCO/H<sub>2</sub>O**

## Objectives

- **Catalysts with high selectivity**
- **Minimize NCO/H<sub>2</sub>O RX in WB PU**

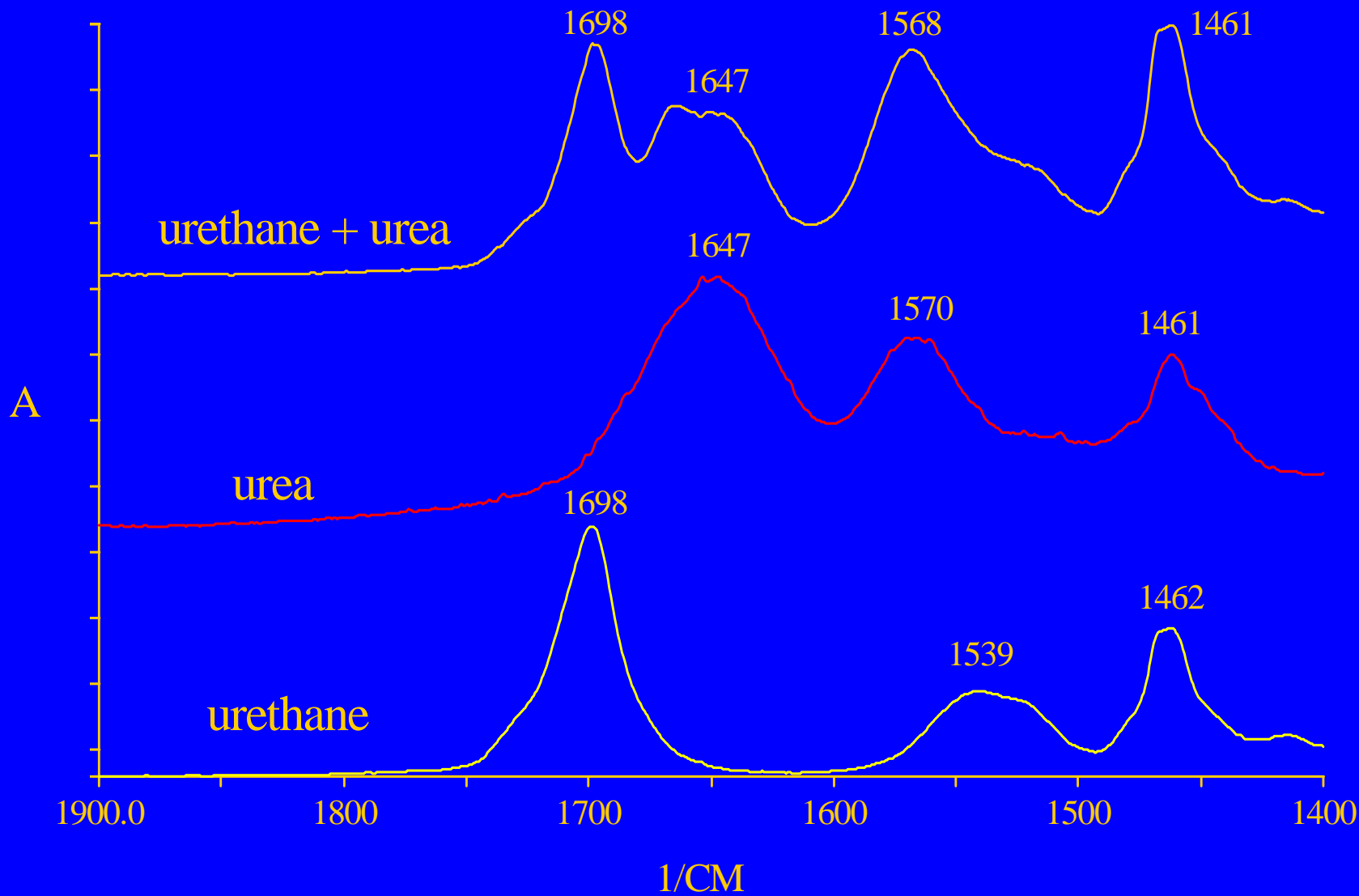
## **Experimental Approaches**

- **FT-IR Selectivity Screening**
- **Evaluation in 2K WB PU**

## FT-IR Studies of Selectivity

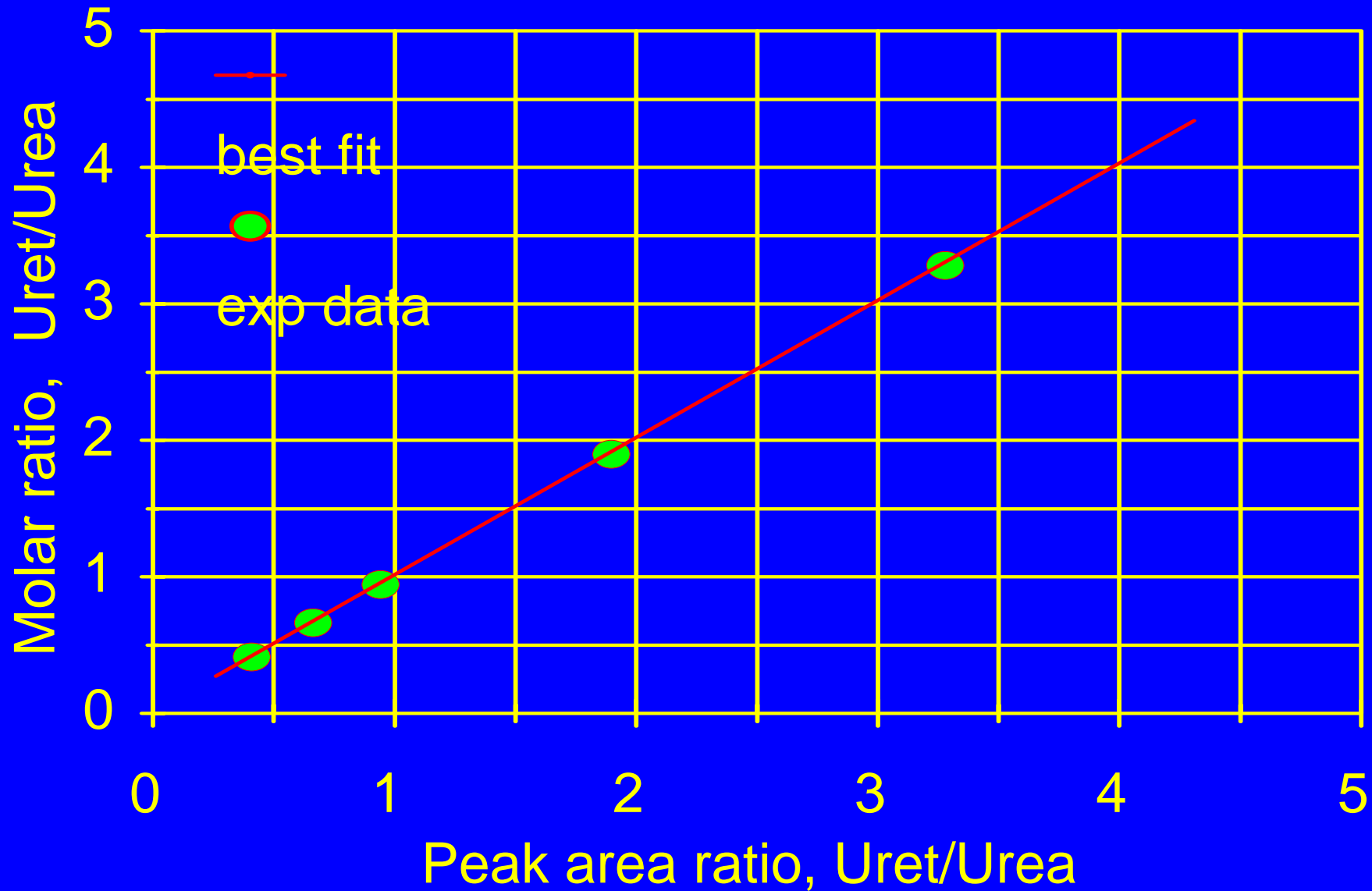
- Homogenous BuNCO/C<sub>8</sub>H<sub>17</sub>OH/H<sub>2</sub>O  
(1.0/ 1.0 / 2.0)
- Relative Selectivity:

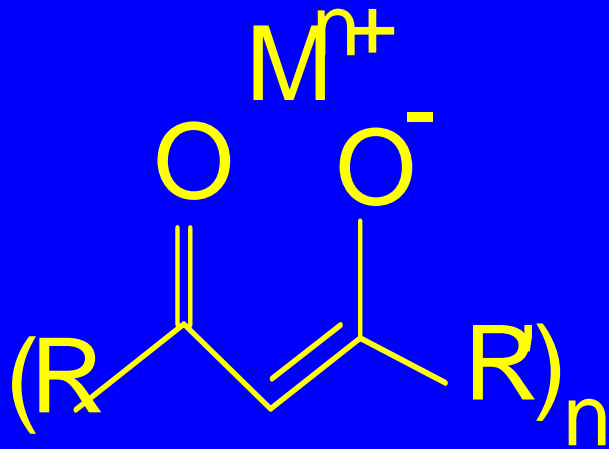
$$S = [\text{urethane}] / [\text{urea}]$$



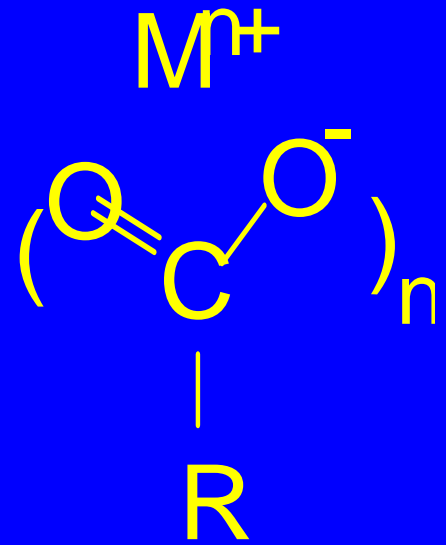
# Calibration Curve

Mole ratio vs. peak ratio

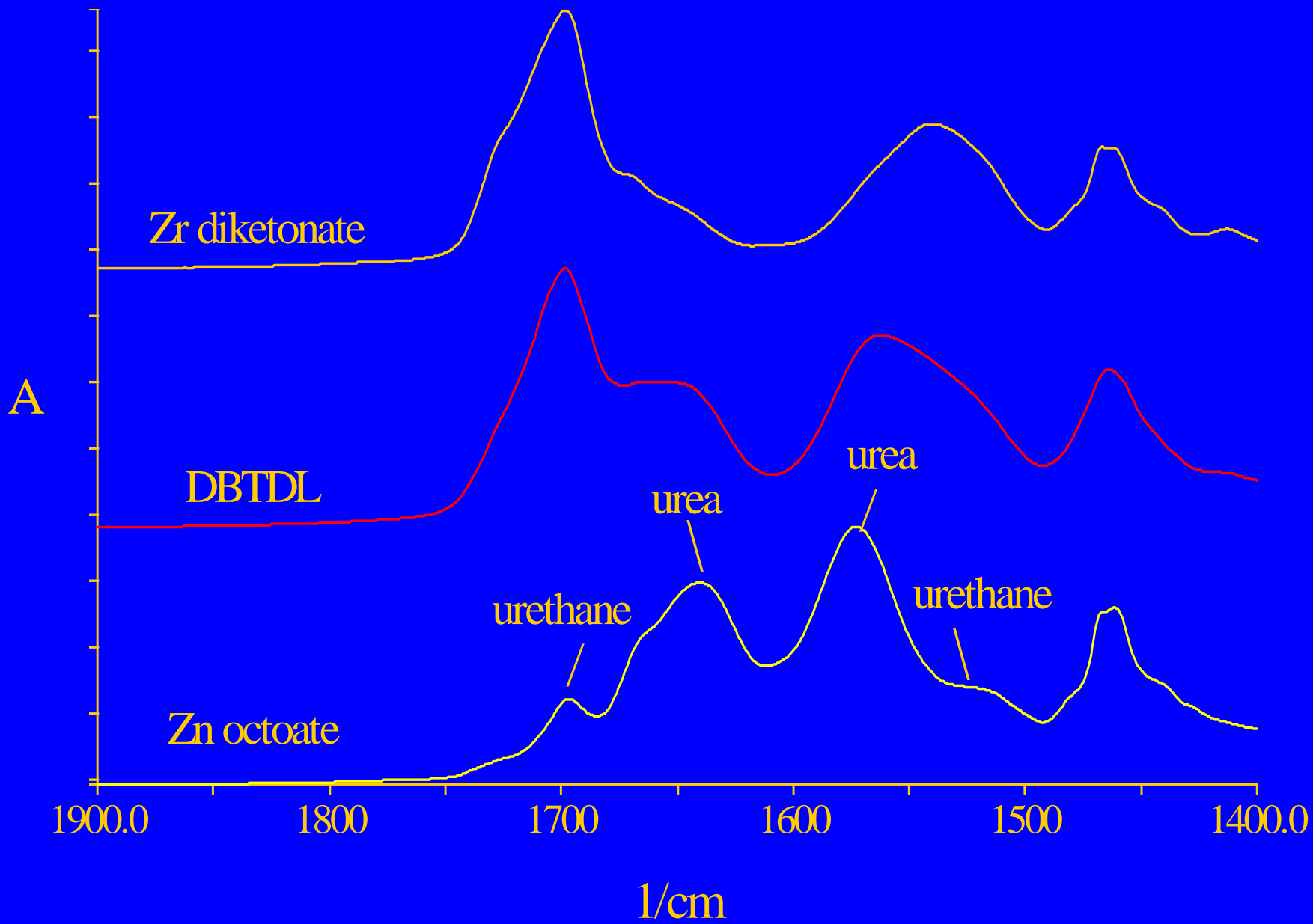




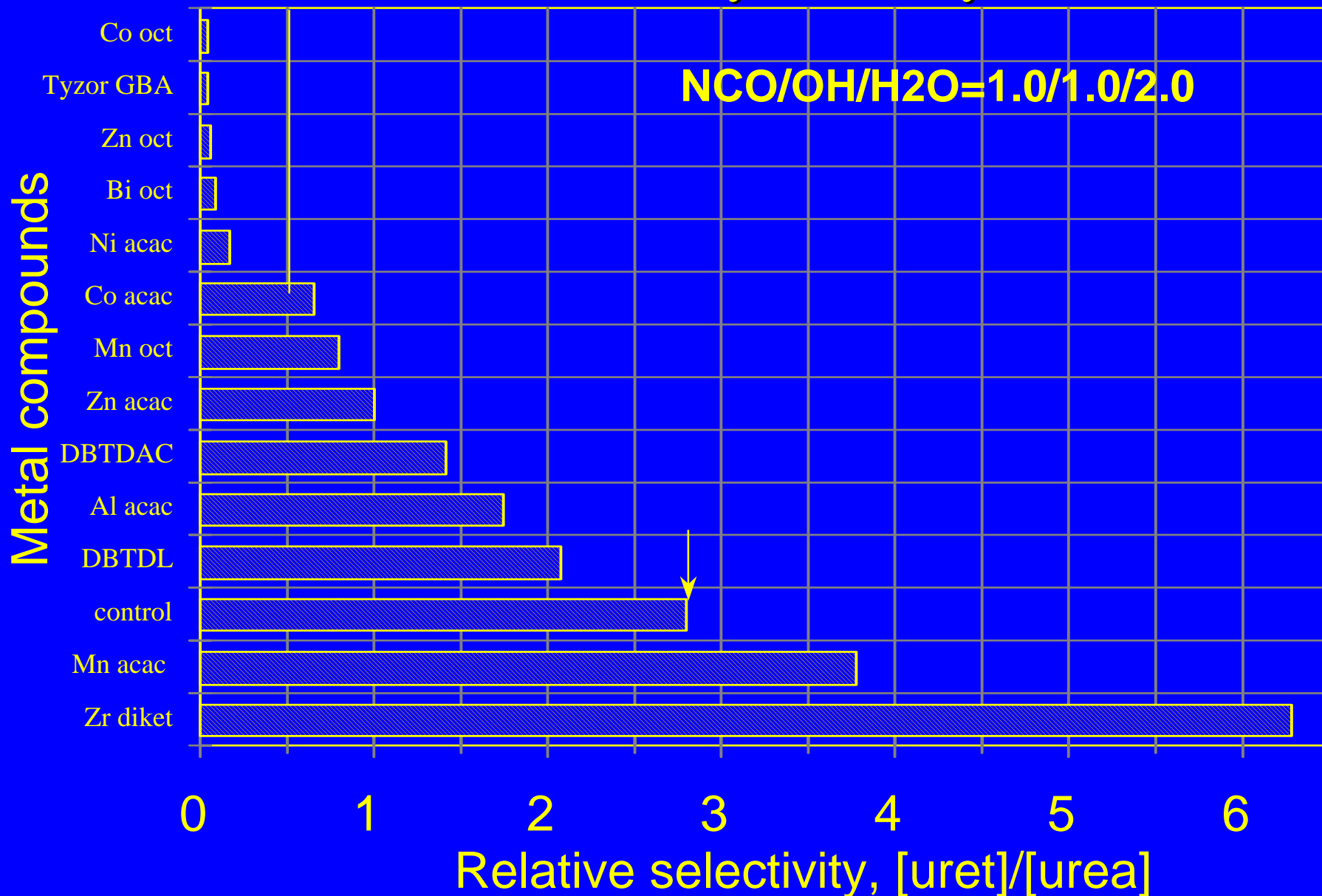
Diketonate

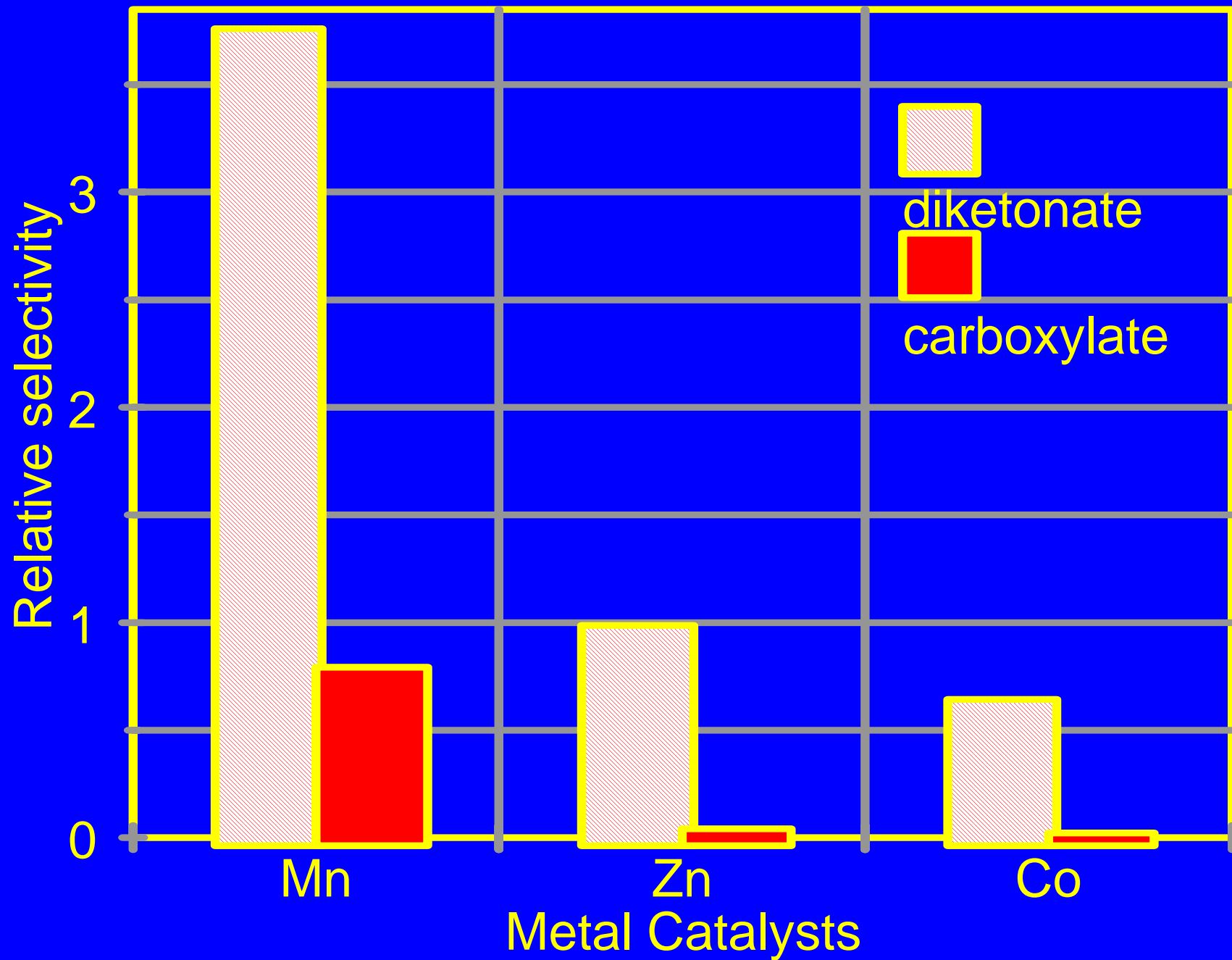


Carboxylate



# Relative Selectivity vs. Catalysts





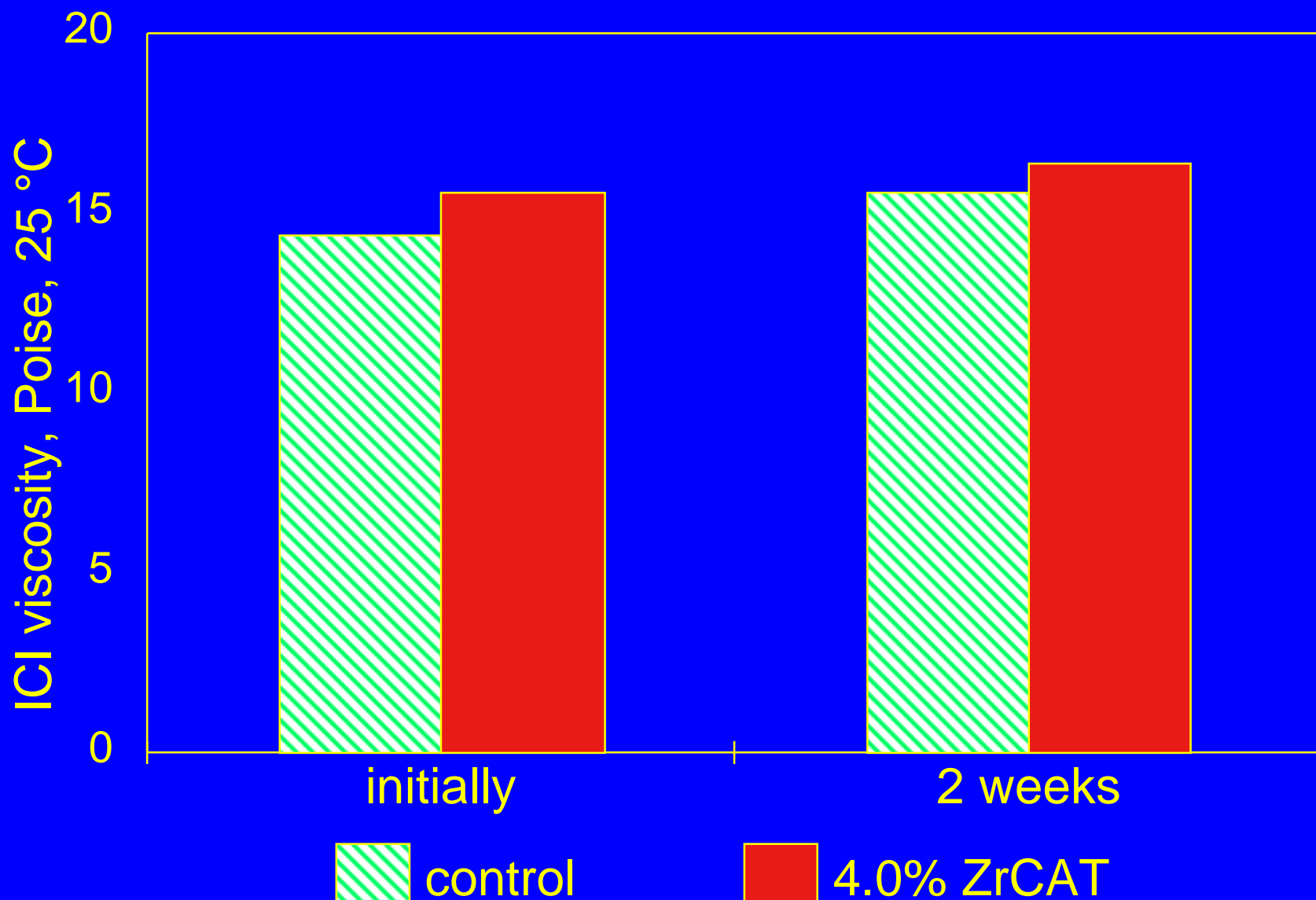
## Properties of ZrCAT (K-KAT XC6212)

<b>Appearance</b>	<b>Clear liquid</b>
<b>Nonvolatile, 60 min at 110 °C</b>	<b>95%</b>
<b>Gardner color</b>	<b>2</b>
<b>Viscosity, 25 °C, cps</b>	<b>100</b>
<b>Specific gravity, 25 °C, g/mL</b>	<b>0.98</b>
<b>Zr metal, %</b>	<b>0.38</b>

## Catalyst Deactivation

- **Hydrolysis**
- **Pigment adsorption**
- **Other interactions**

# Stability of ZrCAT in a HDI trimer, 50 °C



## 2k WB PU with a polyester dispersion

<b>Weight , %</b>	<b>Zr Catalyst</b>	<b>DBTDL</b>	<b>Control</b>
<b>Part A</b>			
<b>Adura 100</b>	<b>41.3</b>	<b>41.3</b>	<b>41.3</b>
<b>Water</b>	<b>9.3</b>	<b>9.3</b>	<b>9.3</b>
<b>Metolat 355</b>	<b>0.2</b>	<b>0.2</b>	<b>0.2</b>
<b>DBTDL</b>	<b>0.0</b>	<b>0.04</b>	<b>0.0</b>
<b>Part B</b>			
<b>HDI Trimer</b>	<b>38.1</b>	<b>38.1</b>	<b>38.1</b>
<b>K-Kat 6212</b>	<b>1.3</b>	<b>0.0</b>	<b>0.0</b>
<b>Water</b>	<b>9.8</b>	<b>11.1</b>	<b>11.1</b>
<b>Total</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>

## **Formulation parameters:**

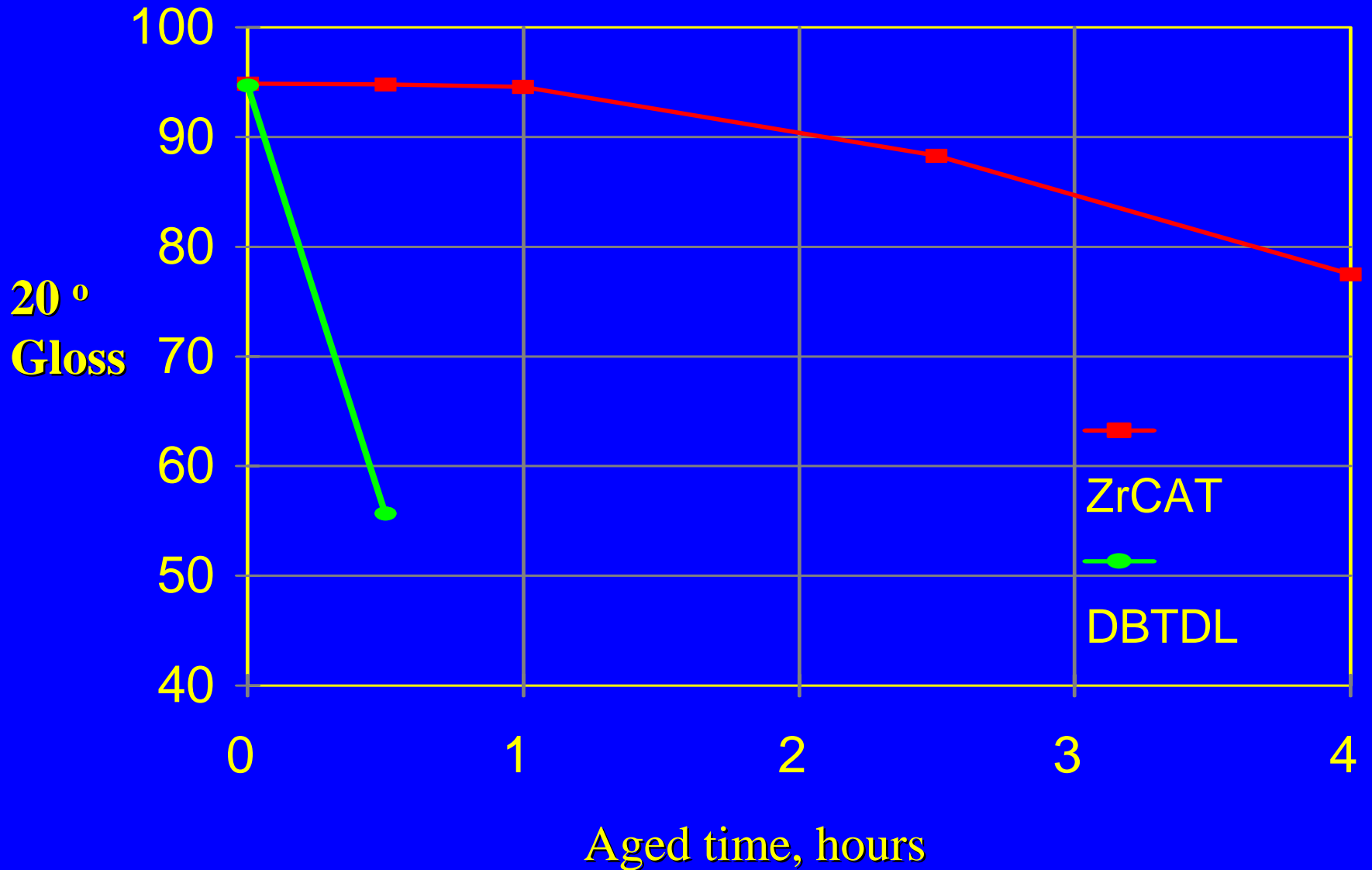
<b>VOC</b>	<b>0 %</b>
<b>Resin solids</b>	<b>67%</b>
<b>NCO/OH</b>	<b>1.3</b>
<b>pH</b>	<b>7.0</b>

## Cure responses, 1 mil on aluminum panel

	Zr catalyst	DBTDL	No catalyst
66 ° F, 23 % RH:			
Surface dry, hrs	3.7	3.5	6
Through dry, hrs	4.7	4.5	8
66 ° F, 70 % RH:			
Surface dry, hrs	4.0	3.8	8
Through-dry, hrs	5.0	4.8	12

# Catalyst Comparison, potlife

2.5 mils DFT at 23% RH & 66 °F



**ZIRC B  
0 HOUR**



**ZIRC B  
4 HOURS**

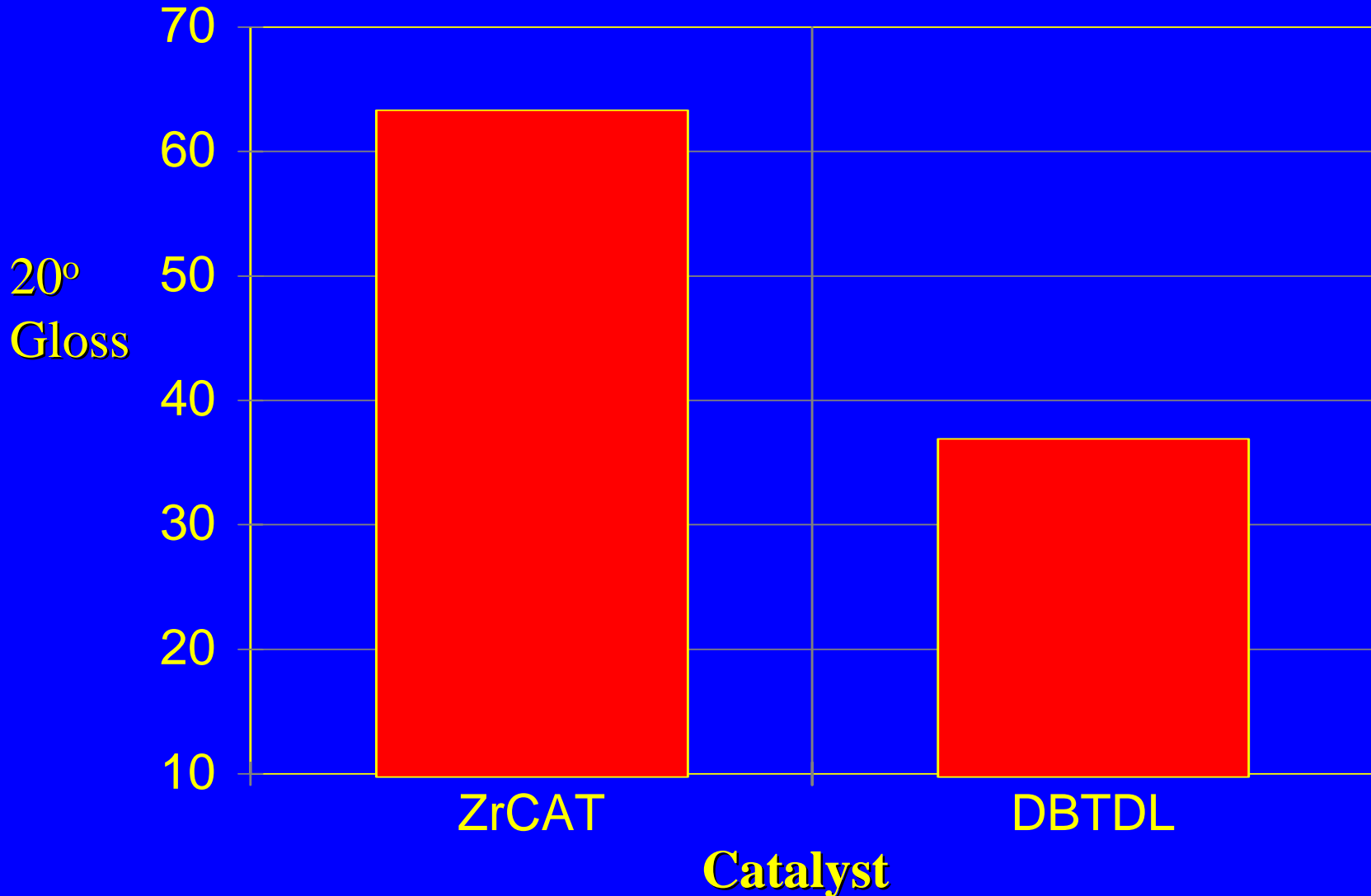


**DBTDL  
0.5 HOURS**



# Catalyst Comparison, Humidity

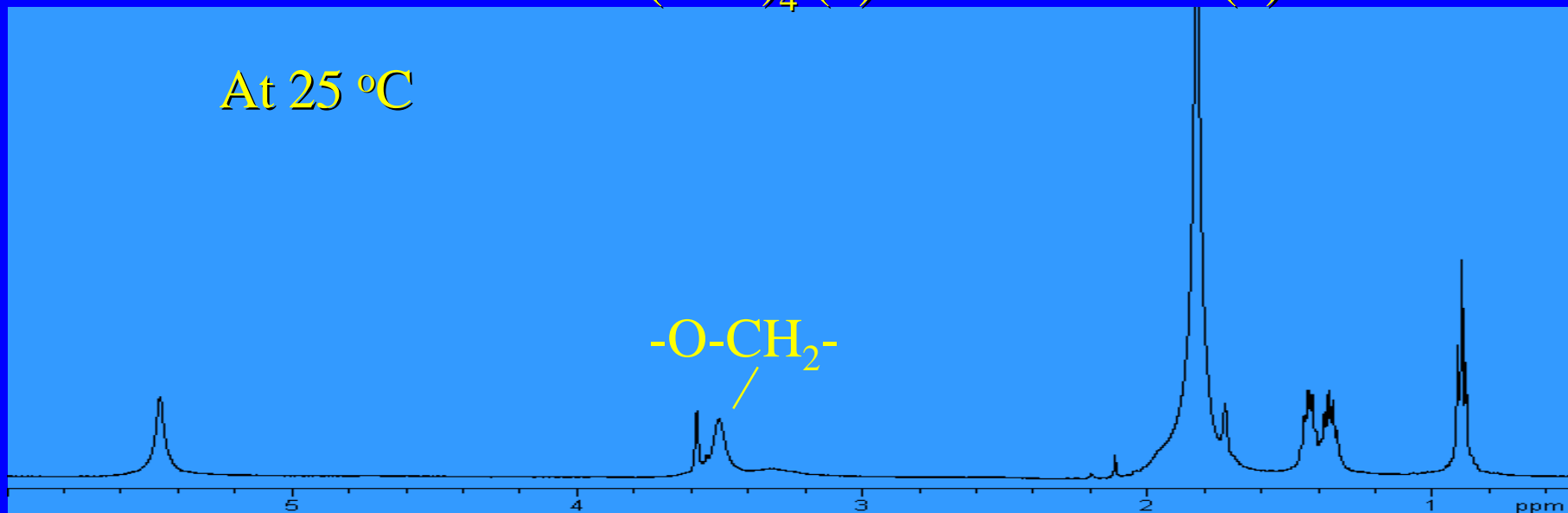
2.5 mils DFT at 70% RH & 66 °F



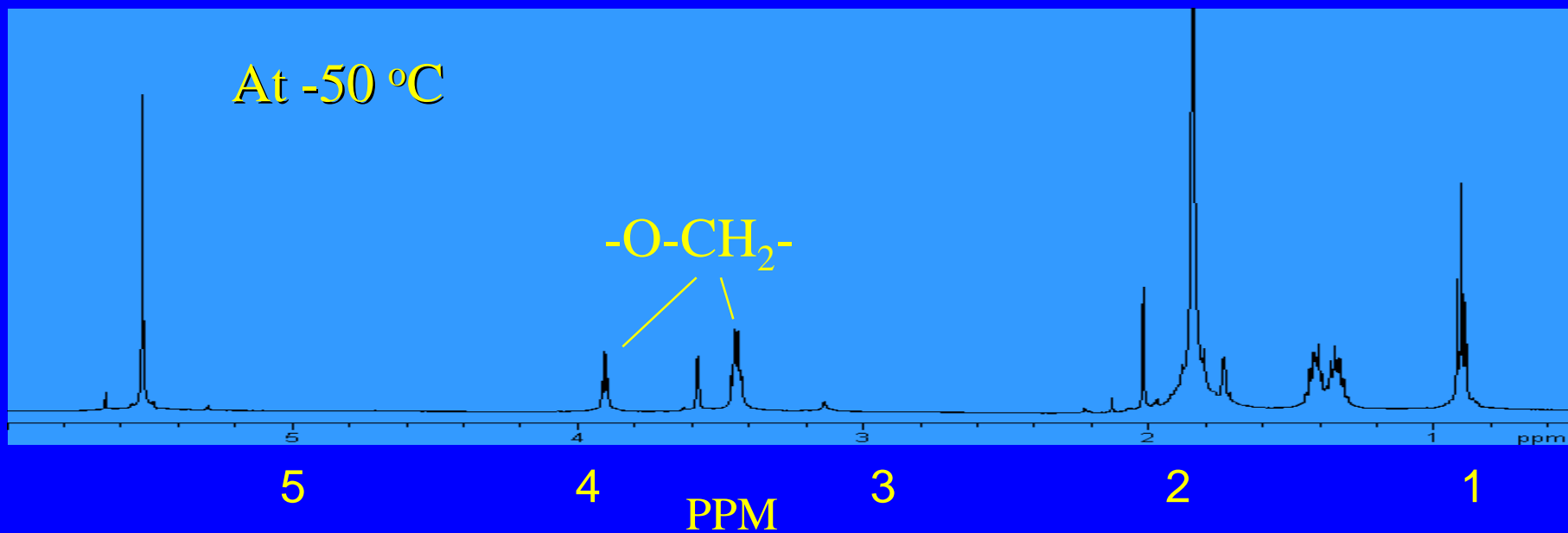


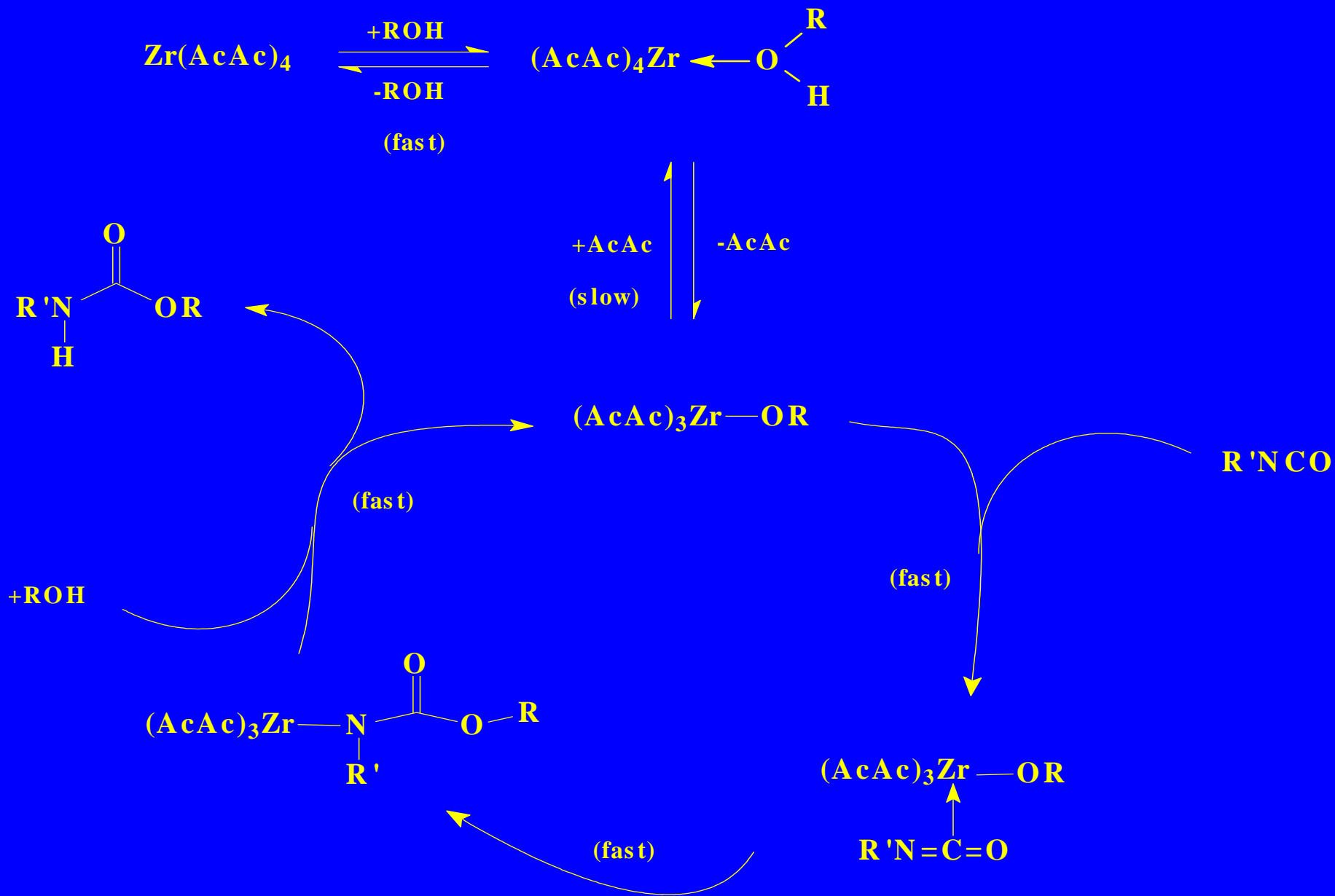
# Proton NMR of $\text{Zr}(\text{acac})_4$ (1) and n-Butanol (3)

At 25 °C



At -50 °C





## Insertion mechanism

## Conclusions

- **Zr diketonates have high selectivity**
- **Less H<sub>2</sub>O RX in WB PU with a Zr catalyst**

# **Acknowledgment**

**David Malkin, John Florio**

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**King Industries, Inc.**

**USM**

