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A Selective Catalyst for 2K WB Polyurethane Coatings

**Z. A. He, W. J. Blank & M. E.
Picci**

King Industries, Inc.



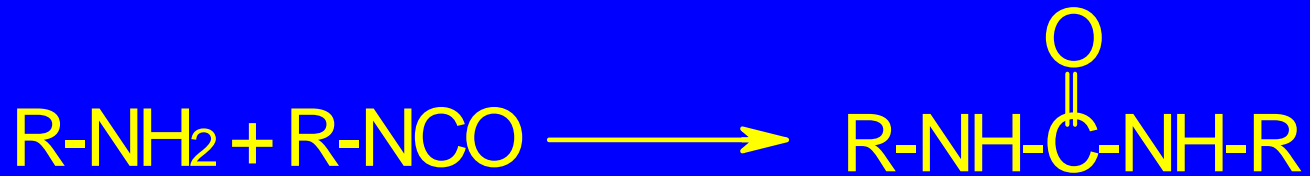
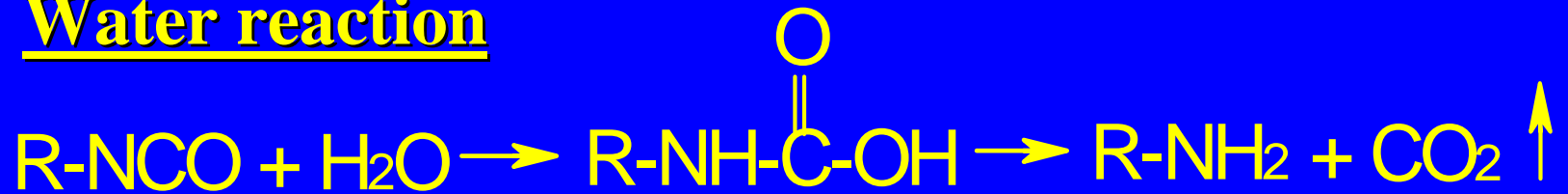
Outline

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

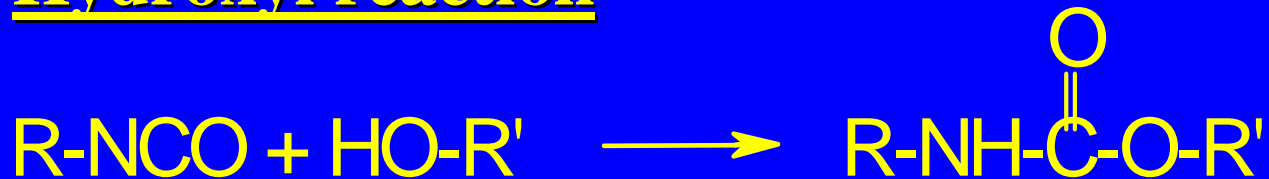
Driving Force for 2K WB PU

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

Water reaction



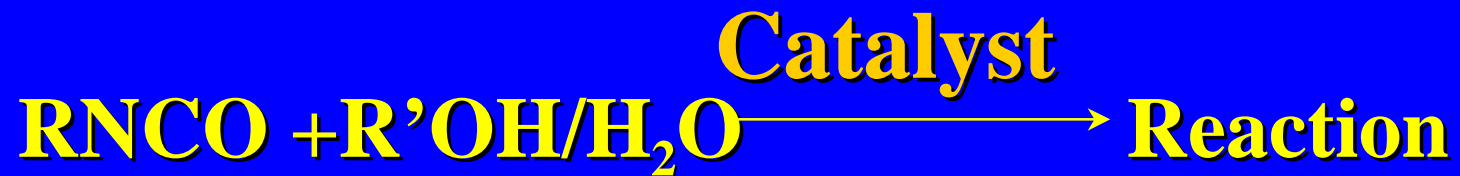
Hydroxyl reaction



Problems of NCO/H₂O

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

A novel chemical approach:



**Control NCO/H₂O reaction
with a selective catalyst**

Previous Studies on Selectivity

- **DBTDL & DBTDCh in diff. solvents**
- **DBTDL, DABCO & Hg on NCO/H₂O**
- **Diff. in amine catalyzed NCO/H₂O**

Objectives

- **Catalysts with high selectivity**
- **Minimize NCO/H₂O RX in WB PU**

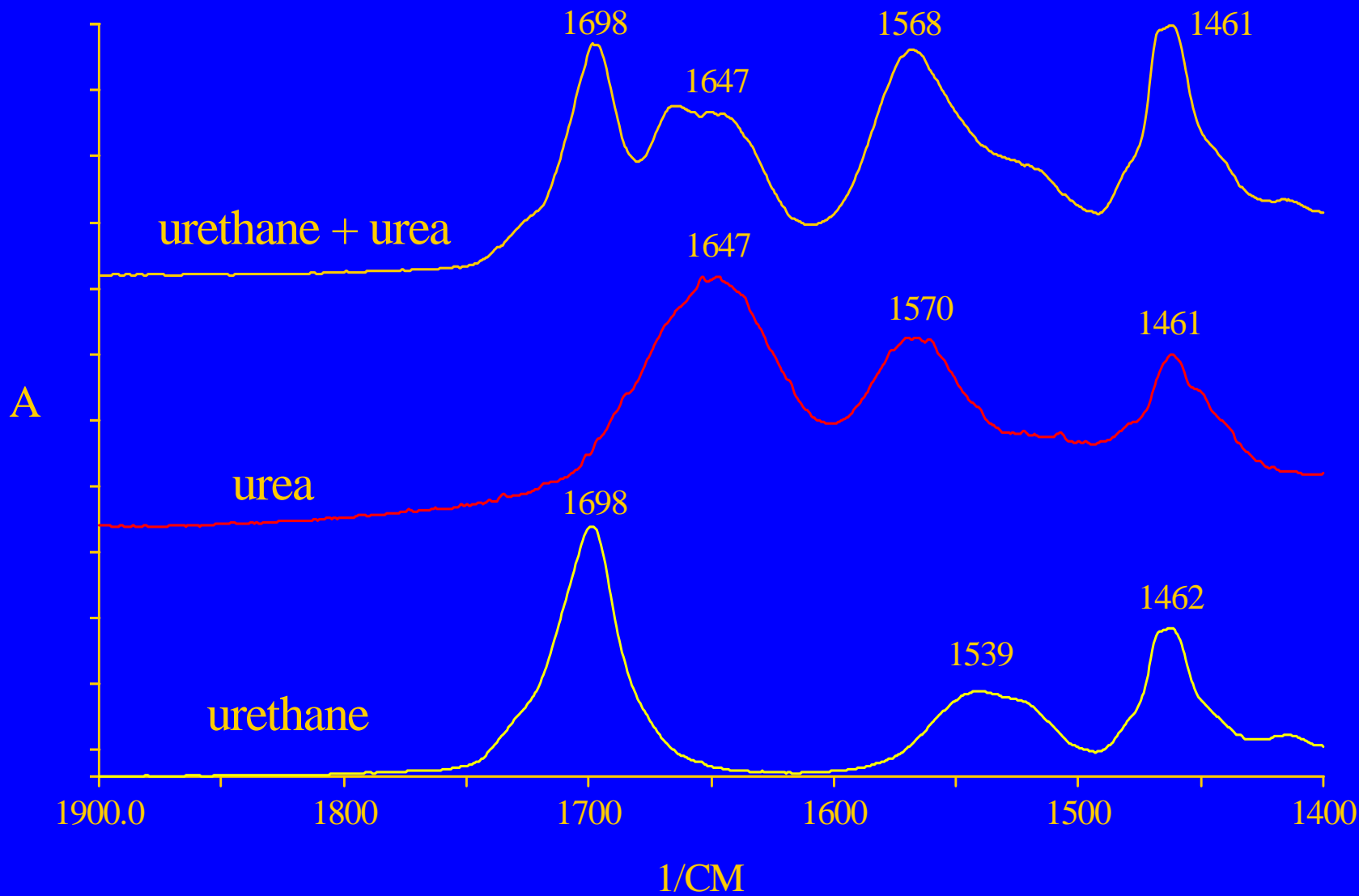
Experimental Approaches

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

FT-IR Studies of Selectivity

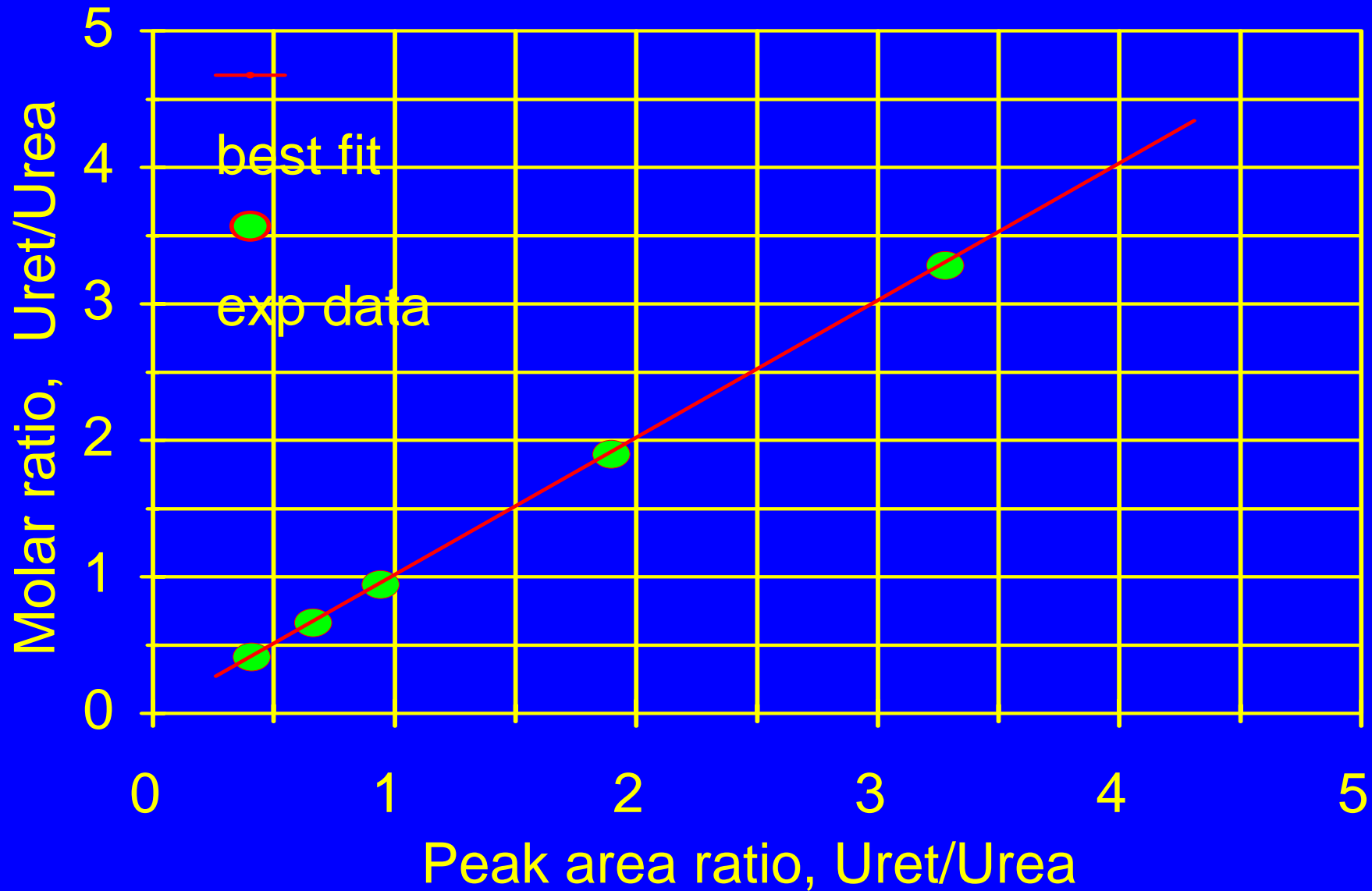
- Homogenous BuNCO/C₈H₁₇OH/H₂O
(1.0/ 1.0 / 2.0)
- Relative Selectivity:

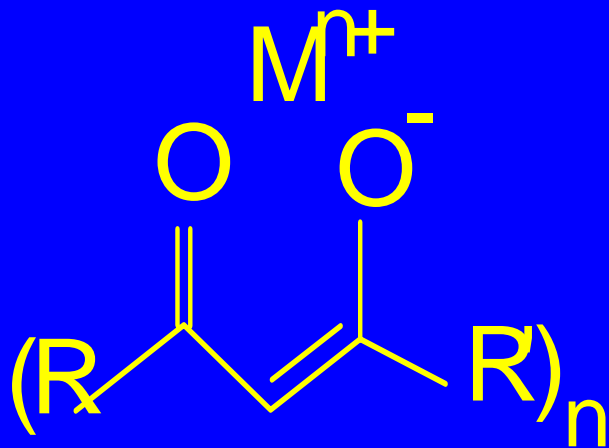
$$S = [\text{urethane}] / [\text{urea}]$$



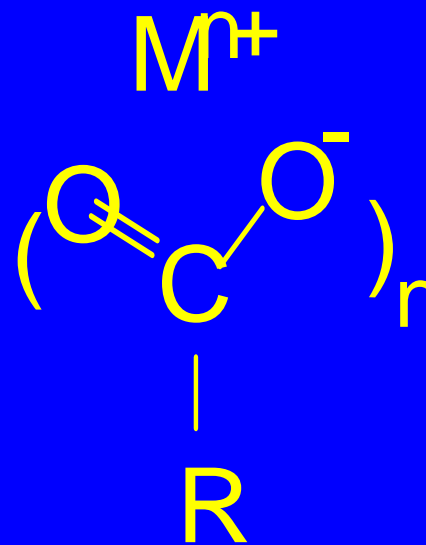
Calibration Curve

Mole ratio vs. peak ratio

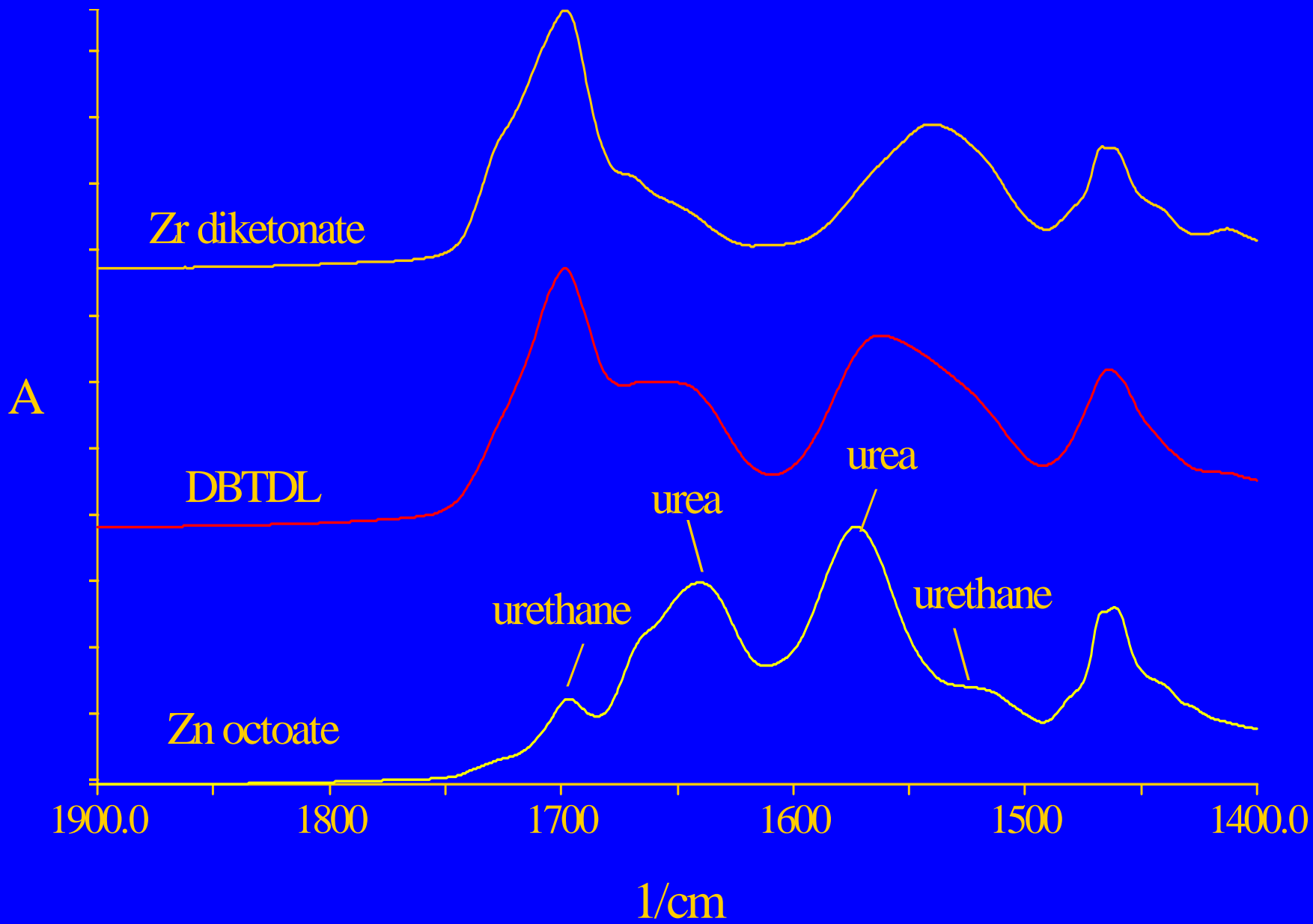




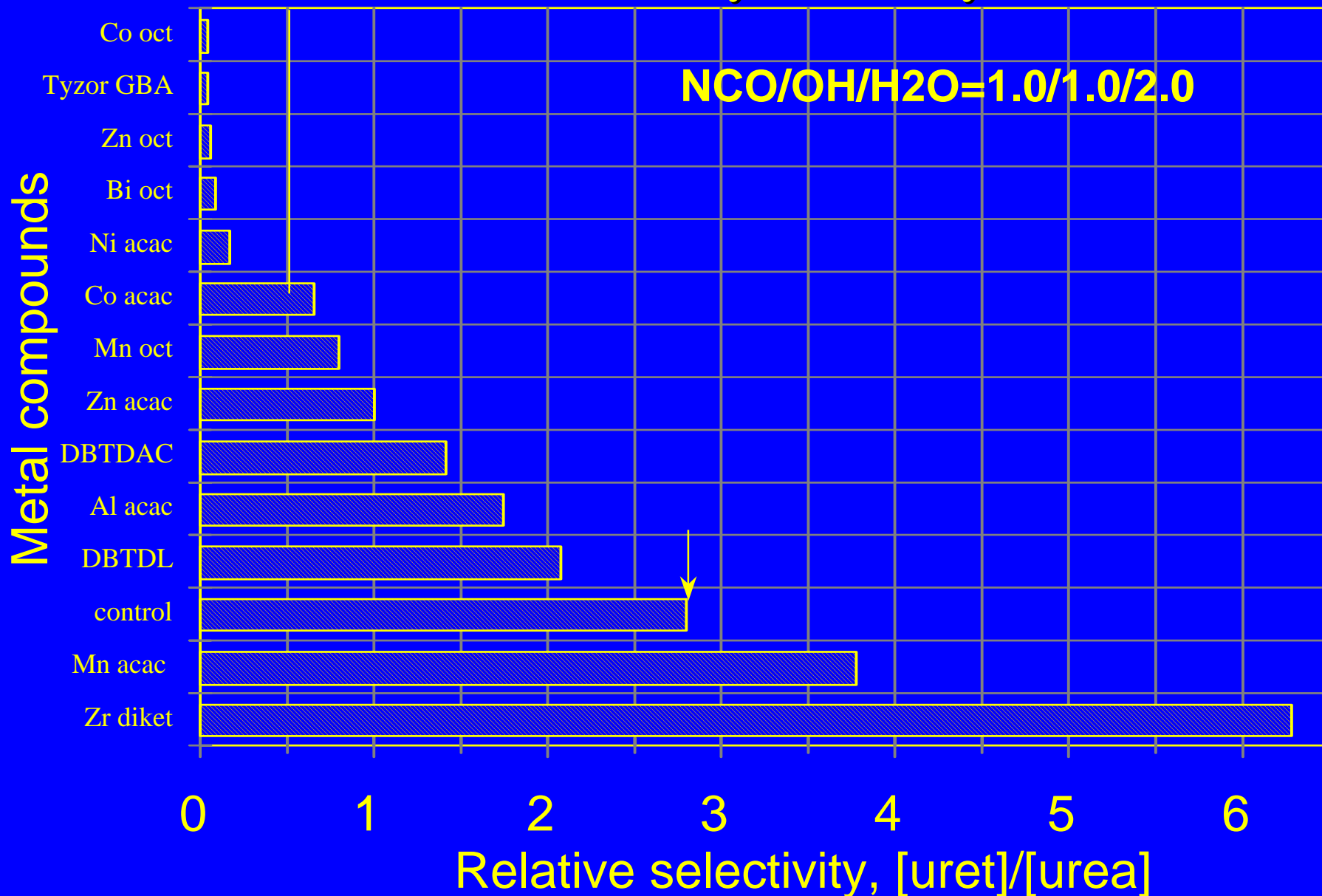
Diketonate

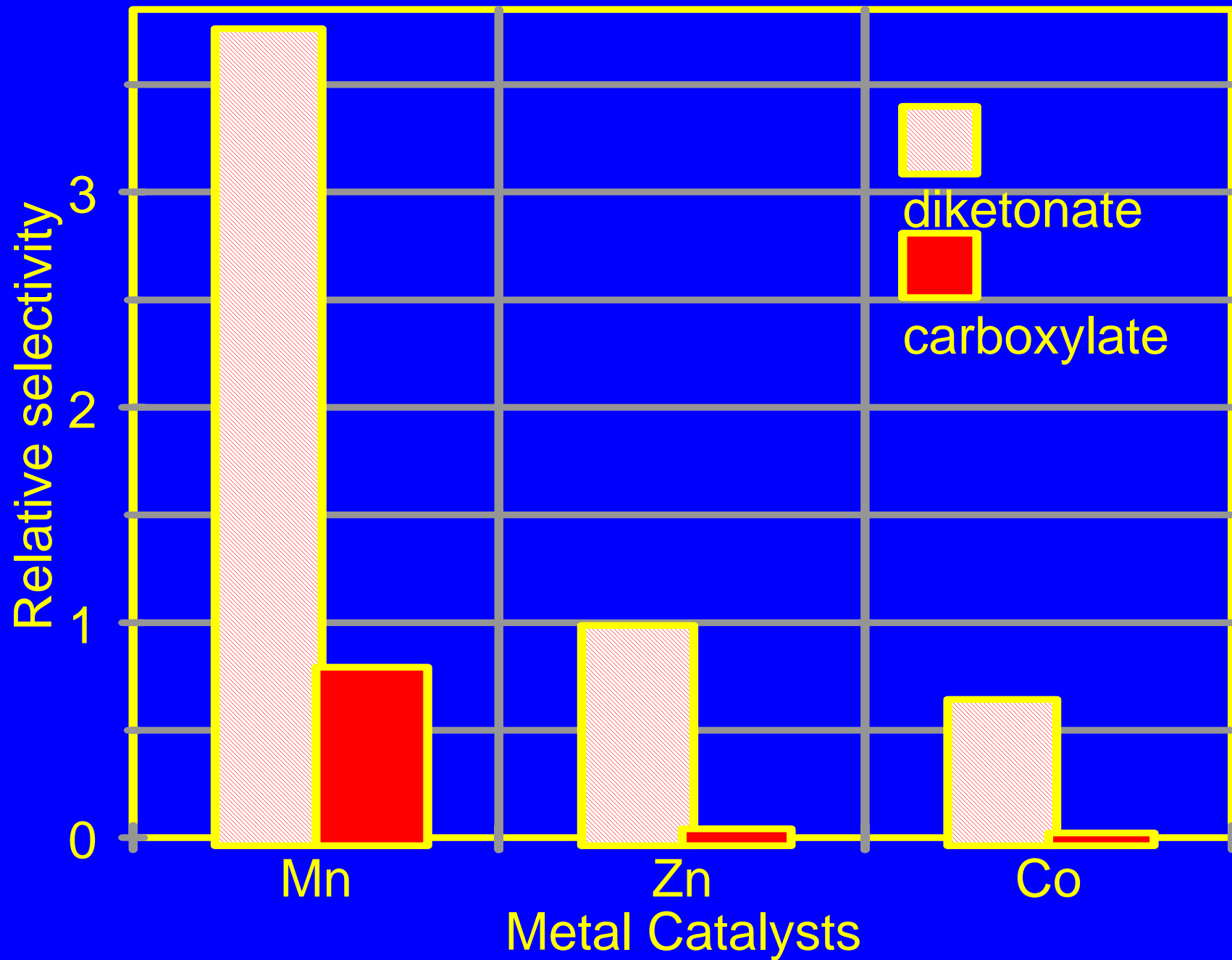


Carboxylate



Relative Selectivity vs. Catalysts





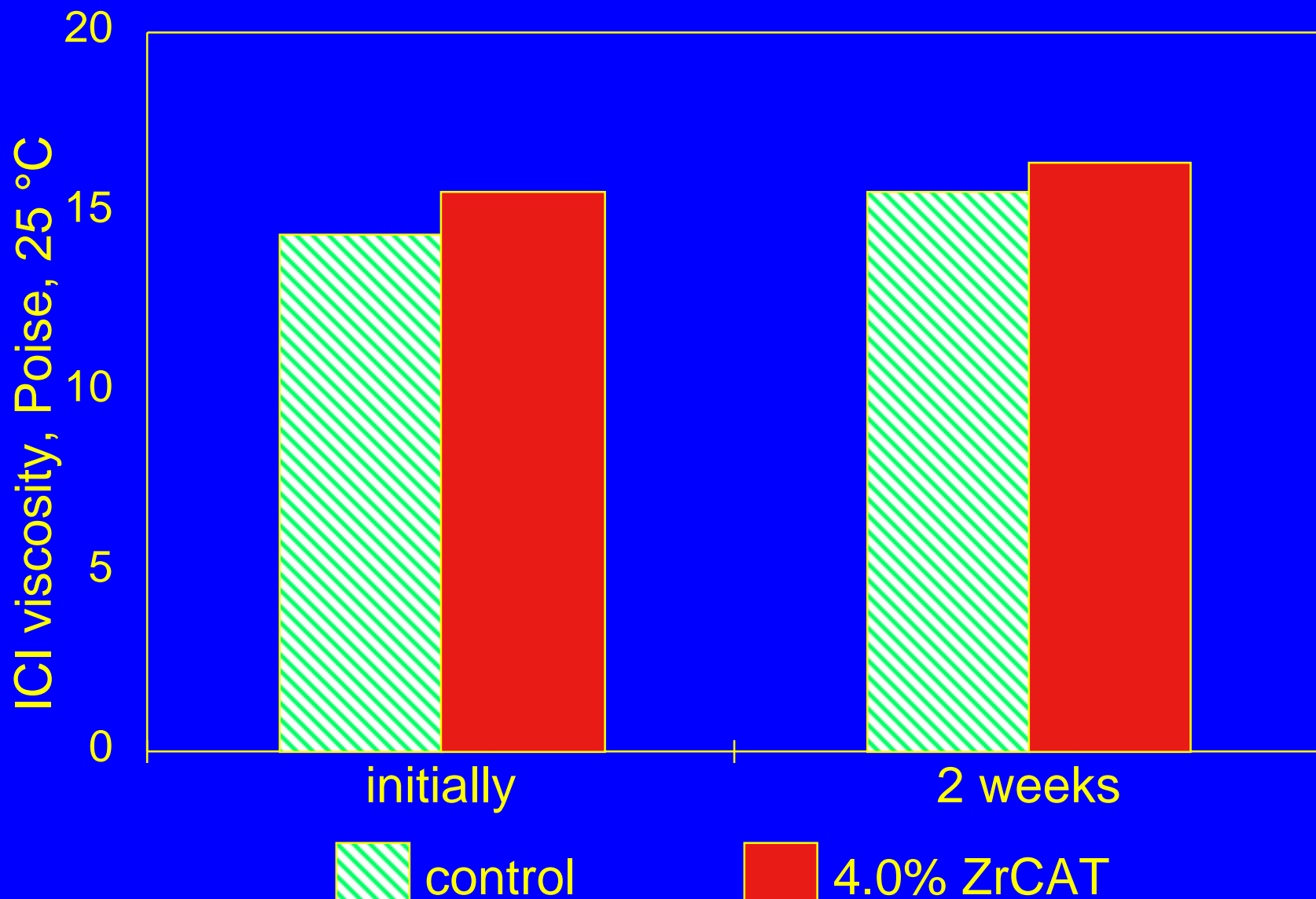
Properties of ZrCAT (K-KAT XC6212)

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

Catalyst Deactivation

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

Stability of ZrCAT in a HDI trimer, 50 °C



2k WB PU with a polyester dispersion

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

Formulation parameters:

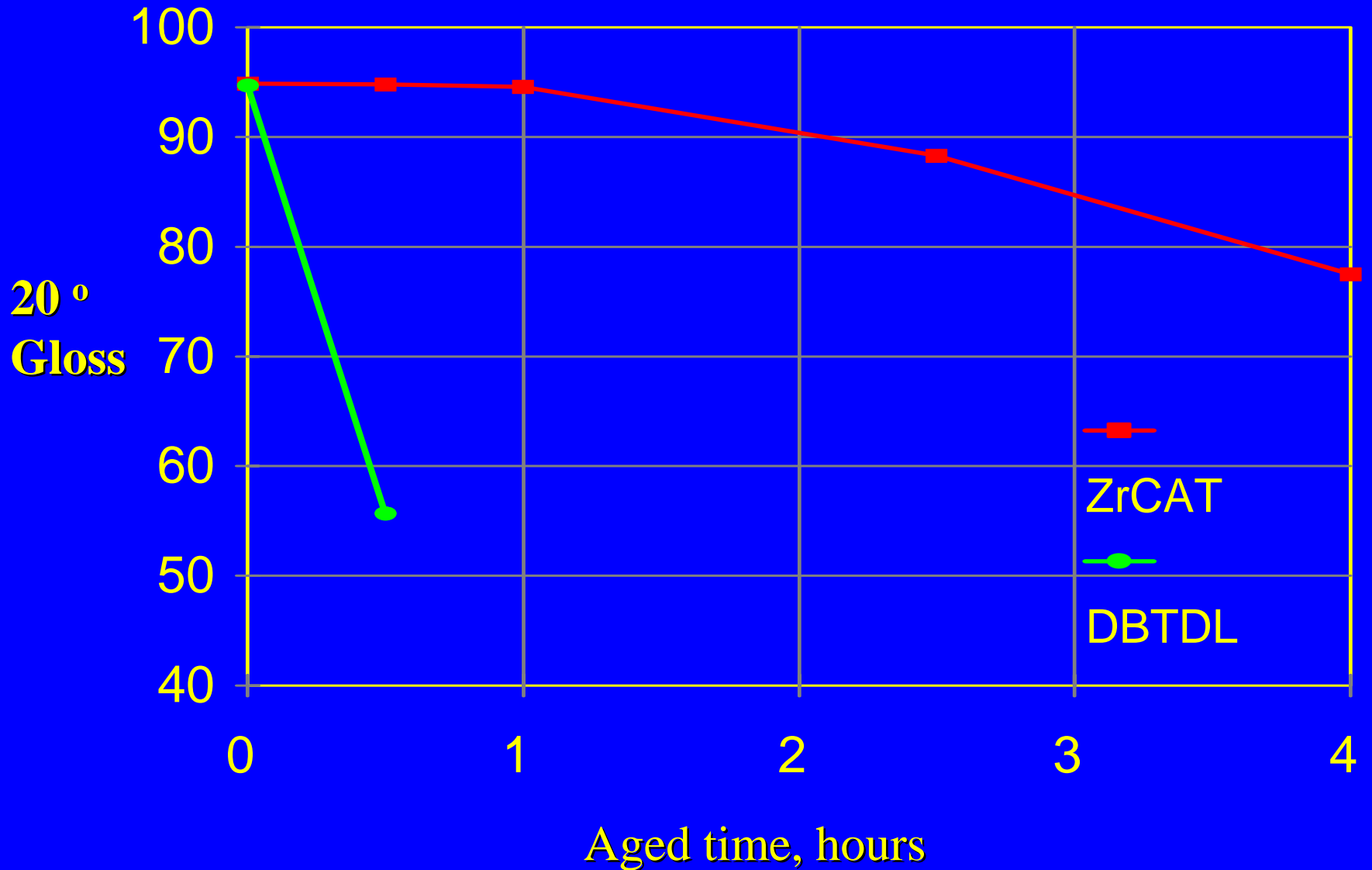
| | |
|---------------------|------------|
| VOC | 0 % |
| Resin solids | 67% |
| NCO/OH | 1.3 |
| pH | 7.0 |

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**

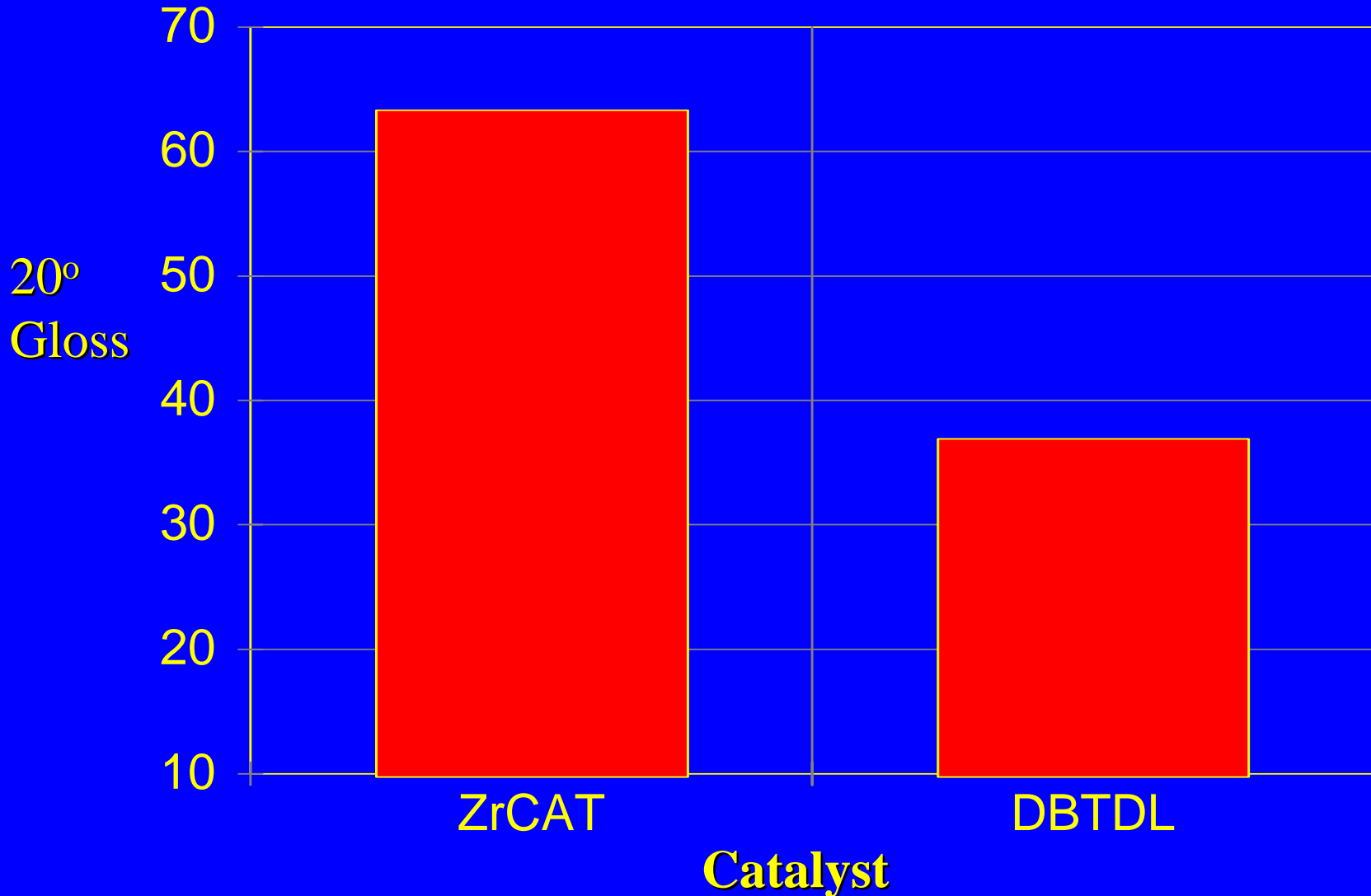


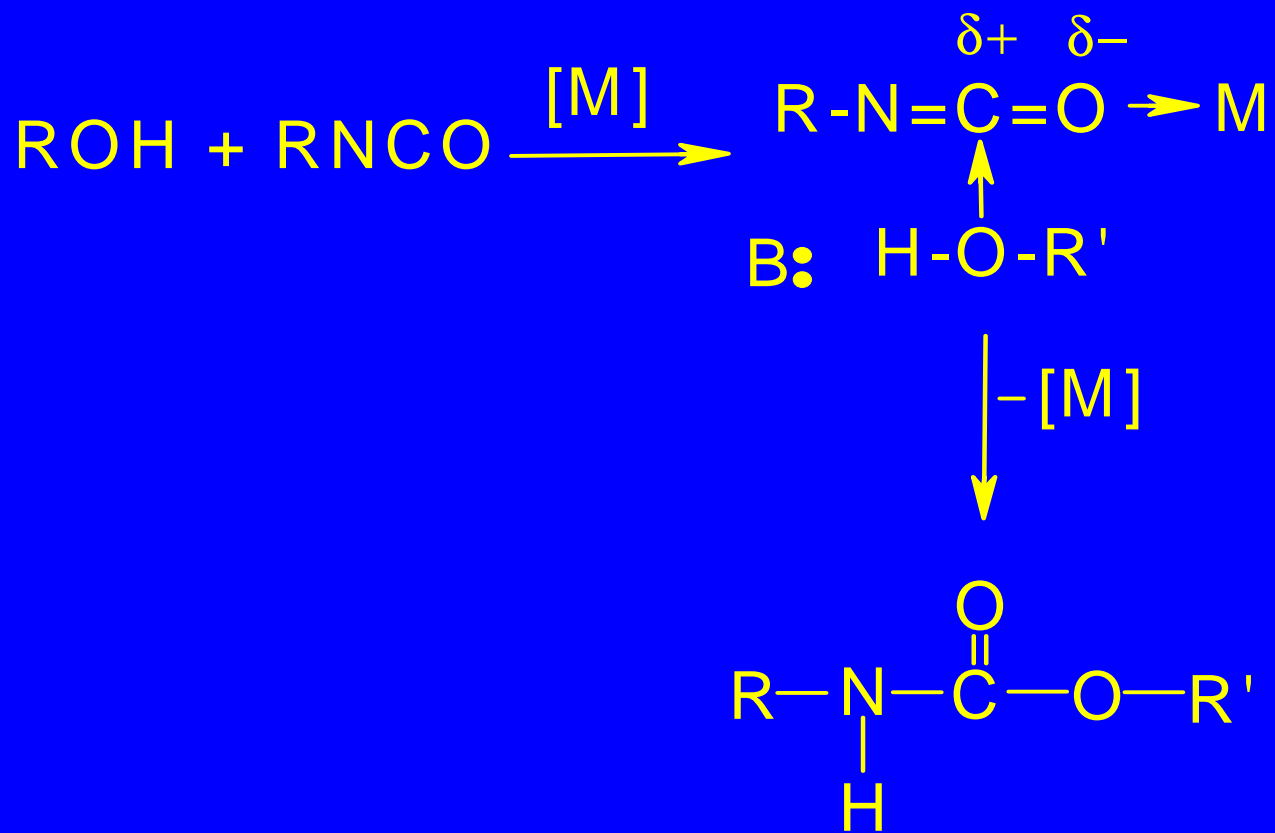
**DBTDL
0.5 HOURS**



Catalyst Comparison, Humidity

2.5 mils DFT at 70% RH & 66 °F

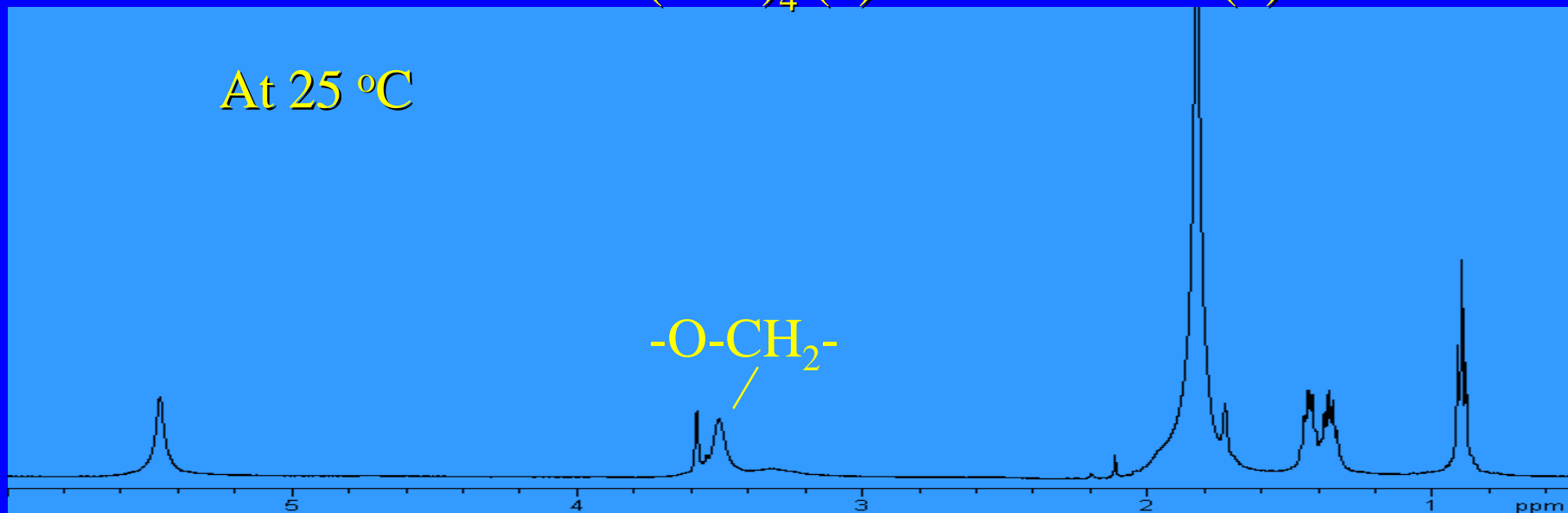




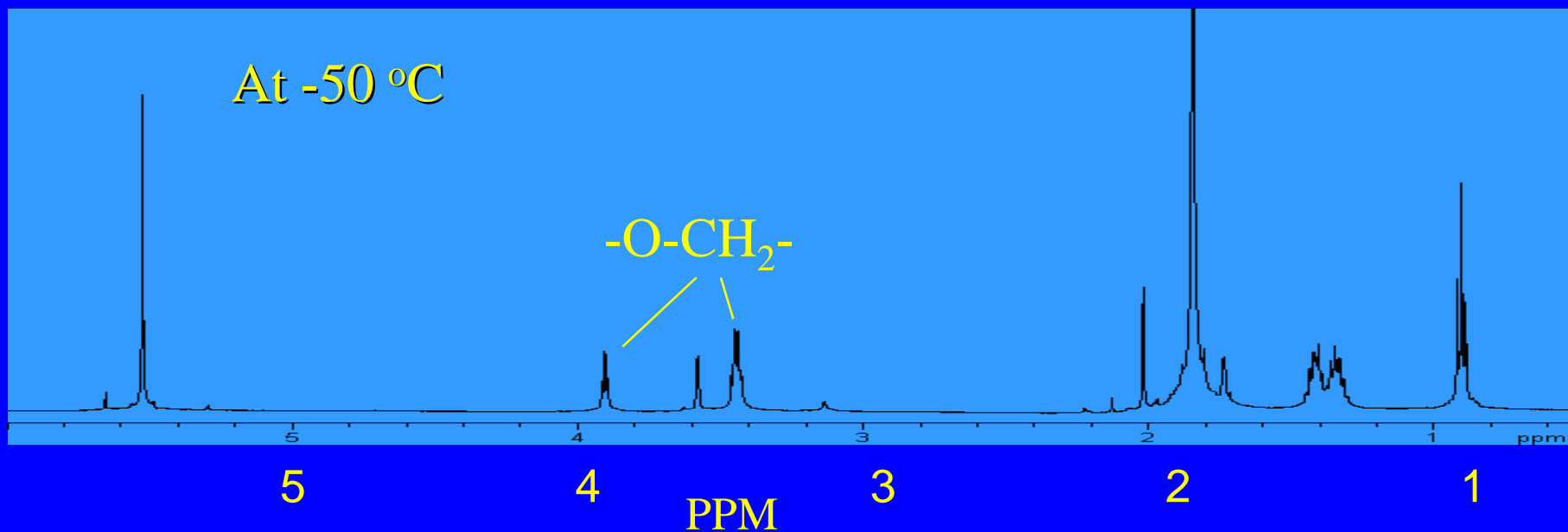
Lewis Acid Mechanism (Tin catalysts)

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

At 25 °C



At -50 °C



Conclusions

- **Zr diketonates have high selectivity**
- **Less H₂O RX in WB PU with a Zr catalyst**

Acknowledgment

David Malkin, John Florio

Ed Hessell, Len Calbo

King Industries, Inc.

USM

