

100

METAL-BASED CATALYSTS FOR POLYURETHANES











A Sustainable Approach to Technology

Patcham FZC is a global manufacturer of specialty additives headquartered in the United Arab Emirates. Since its inception, Patcham has steadily grown to become a leading supplier of metal carboxylates and specialty additives for Paint & Coatings, Inks, PVC, Composites and Polyurethane. We also manufacture a range of tin based and tin free catalysts for various end use industries.

The company's Pat-Add range of coating additives includes driers, wetting & dispersing agents, defoamers, slip & leveling agents, rheology modifiers. All our products are APEO free and many are produced from green raw materials. Several are designed to enable our customers to make products that are low VOC or VOC free.

Patcham has a strong manufacturing and R&D infrastructure that enables rapid transition from concept to products. The company has strategically located technical service laboratories, offices and representatives around the world to provide efficient customer service. In addition, a well-developed robust supply chain network enables us to deliver our products and services to customers around the globe with minimal lead-time.



General Information

Polyurethanes (PU) are one of the most versatile plastic materials.

There are several chemical reactions that occur in the formation of Polyurethane PU and Polyisocyanurate PIR products that require the assistance of catalysts. Blow reaction is important for many foams but produces unwanted gassing in other systems.

Blow reaction is important for many foams but produces unwanted a Gel reaction is the defining reaction for all urethanes. Trimerization is required for the production of rigid foams.

These reactions occur readily at temperatures above 110°C. However, at room temperature without a catalyst, they are slow, taking days.

	Isocyanate reaction with	
FAST	water	bl
MEDIUM	polyols	ge
SLOW	isocyanate	рс

Catalysts exert a considerable influence on PU structures and its end properties by changing the relative rate of these primary chemical reactions.

Catalysts have a tendency to catalyze several of these reactions at once, although to differing degrees, and their individual action can be highly temperature and time dependent.

A mix of catalysts is often required to achieve a critical balance between these reactions in order to achieve the desired end product properties and workability.

Additions of metal-containing catalysts, in concentrations that can be measured in ppm, have a profound effect on the rate of reactions and can produce synergy with tertiary amine catalysts.

Catalyst deactivation can be a function of water content in the PU system and thus hydrolytic stability of the catalyst is also an important formulating consideration.

PU/PIR Catalysts are mainly tertiary amines and metal-containing compounds

Princi	Principal Reactions		Amines	Metal-Based	Amines	Metal-Based Catalysts			
1 1110	particulation	Product		Catalysts	Bad smell	Low odor			
Blow reaction	NCO/H2O	Urea + CO₂	Ctrong	Weak	Corrosive	Non-corrosive			
BIOW reaction	Isocyanate/water	Uled + CO2	Strong	vveak	High pH	Neutral			
	NCO/OH				Toxicity issues	Many have very low toxicit			
Gel reaction		Polyurethane	Strong	Strong	Strong	rong Very Strong	y Very Strong	Instability with acid treated pigents	Non-reactive towards acid t
	Isocyanate/polyol				Deactivation of HFO blowing agents	Stable with HFO blowing age			
Trimeries	NCO/NCO	Polyisocyanurate	Weak	Very Strong	Low Flash Point	Many have high flash point			
Trimerization	Isocyanate/isocyanate		weak	very sciolig	End product discoloration	Several have very low color			



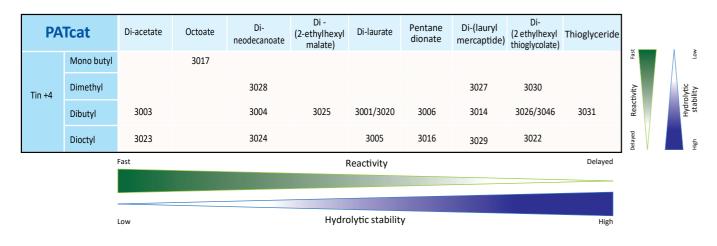
Metal Catalysts for Polyurethanes

low reaction el reaction olymerization of which Trimerization is the most important

Metal based catalysts are far more desirable than amines

Tin Based Catalysts

Tin based gel catalysts cover a rage of activity from Fast Acting to Delayed Action and varying degrees of hydrolytic stability.



Generally tin catalysts that demonstrate delayed action tend to have better hydrolytic stability.

PATcat Tin Catalyst					
PATcat 3017	Monobutyltin trioctoate	19.0%			
PATcat 3028	Dimethyltin dineodecanoate	23.5%			
PATcat 3027	Dimethyltin dilauryl mercaptide	20.5t%			
PATcat 3030	Dimethyltin di (2-ethylhexyl thioglycolate)	19.0%			
PATcat 3003	Dibutyltin diacetate	33.0%			
PATcat 3004	Dibutyltin dineodecanoate	20.0%			
PATcat 3001	Dibutyltin dilaurate	18.0%			
PATcat 3020	Dibutyltin dilaurate (lower crystallization temperature)	18.0%			
PATcat 3014	Dibutyltin lauryl mercaptide	18.0%			
PATcat 3026	Dibutyltin di (2-ethylhexyl thioglycolate)	18.0%			
PATcat 3046	Dibutyltin di (2-ethylhexyl thioglycolate)	2.0%			
PATcat 3025	Dibutyltin di (2- ethylhexyl maleate)	17.0%			
PATcat 3006	Dibutyltin acetyl acetonate	27.0%			
PATcat 3018WB	Dibutyltin dilaurate	1.8%			
PATcat 3031	Dibutyltin thioglyceride	26.5%			
PATcat 3023	Dioctyltin diacetate	26.0%			
PATcat 3024	Dioctyltin dineodecanoate	17.0%			
PATcat 3005	Dioctyltin dilaurate	16.0%			
PATcat 3022	Dioctyltin di (2-ethylhexyl thioglycolate)	15.0%			
PATcat 3029	Dioctyltin di (lauryl mercaptide)	15.5%			
PATcat 3016	Dioctyltin acetyl acetonate	21.0%			



Trimerization reaction in the PIR industry is essential for the Trimerization is normally the slowest of the isocyanate reactions and formation of rigid closed cell structures that impart dimensional requires catalysts to increase the rate of production and yield of strength and improved insulation properties to the end products. trimerized material:

PATcat 5000 series catalysts can be used as the sole catalyst in PIR systems.

They provide catalysis for the Blow, Gel and Timeization reactions.

Variations in system formulations and production equipment place different demands on the catalyst such as viscosity, OH and water content.

Metal	Anion	Carrier Diluent*	Catalyst strength Metal content %wt/wt**	Water content ⁺	Typical OH value	Typical viscosity ⁺⁺ (Cp) at 25°C	PATcat
			15.0	5.0% max	525	3500	5001
		DEG	15.0	3.5% max	460	7000	5003
	Octoate		10.0	2.0% - 4.0%	700	1200	5011
		MEG	15.3	3.0% - 4.0%	660	3500	5016
		MEG	15.0	9.5% - 10.5%	965	550	5012
			15.0	5.5% max	910	350	5005
sium		DEG	13.2	2.0% max	815	350	5008
Potassium	Acetate		10.0	5.5% max	1060	150	5004
		Acetate	18.0	3.0% - 4.0%	1130	200	5018
			15.3	1.0% max	1100	150	5019
			15.0	3.0% - 5.0%	1290	75	5007
			13.0	2.7% - 3.5%	1340	100	5013
			10.0	3.0% - 5.0%	1530	50	5006
	Neodecanoate	DEG	10.0	3.0% - 5.0%	700	3500	5010
	Propionate	MEG	14.0	4.0%-5.0%	980	120	5020

Smooth Rise Profile Catalyst						
Mixture			3.0% - 5.0%	790	250	5022

Economical Potassium Octoate 15 % Alternative						
Mixture			2.0% - 4.0%	820	250	5101

* DEG gives lower OH values (less unwanted consumption of isocyanate). MEG gives lower viscosity for ease of handling. ** Higher metal content affords lower dosage and better economy.

+ Higher water content gives lower viscosity for ease of handling but increases the OH value. ++ Lower Viscosity improves ease of handling.



Trimerization Catalysts for PIR Applications

Patcham produces a wide range of amine free trimerization catalysts to meet those needs:

PATcat 4202

Tin-Free Replacement for Stannous Octoate in PU Foams

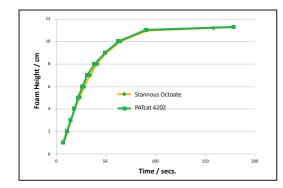
Stannous octoate is commonly used along with tertiary amines in the production of PU foams.

Stannous Octoate	PATcat 4202
 Tin has toxicity issues 	► Tin - free
 Contains Octoate (2 Ethyl Hexanoic Acid) 	2 Ethyl Hexoic acid – free
 Poor Hydrolytic Stability 	 Good Hydrolytic Stability
 Cold Flow problems 	 Very little shrinkage

Performance test results in Flexible and High Resilience Foam

Flexible Foam	Stannous Octoate	PATcat 4202
Polyol 3000	100.0	100.0
33LV	0.3	0.3
Silicon surfactant	1.1	1.1
Water	4.5	4.5
Stannous Octoate	0.2	
PATcat 4202		0.4
TDI (Index 114)	59.9	59.9

Top of the cup (sec)	44	42
Rise time (sec)	115	113
Foam height (cm)	16.9	17
Tack free (Hr:Min)	2:00	1:45
Peak exotherm temp °C	52.4	51.4
Remarks	Shrinkage	

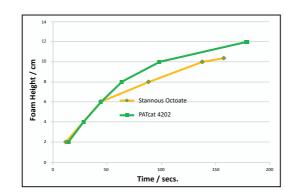




Stannous Octoate PATcat 4202

PATcat 4202 better performance and without the detriments.

HR Foam	Stannous Octoate	PATcat 4202
Polyol for HR Foam	100.0	100.0
Water	2.77	2.77
Cross linker	2.90	2.90
Surfactant	1.10	1.10
Tertiary amine catalyst	0.12	0.12
Stannous Octoate	0.04	
PATcat 4202		0.08
		
TDI (Index 105)	33.00	33.00
Top of the cup (sec)	58	58
Rise time (sec)	142	143
Foam height (cm)	14.6	14.9
Tack free (Hr:Min)	1:30	1:30
Peak exotherm temp °C	52.8	53.3





Patcham produces tin and tin-free catalysts fo including HFOs

Patcham Tin Catalysts



PATcham Tin-Free catalysts for PU Spray Foam:

Enhanced Bismuth Catalyst	Typical Dosage			
PATcat 4012	0.5			
PATcat 4020	0.75			
PATcat 4009	1.0			
PATcat 4031	1.5			
 Improved Hydrolytic Stability Improved shelf stability with HFO blowing agents 				

Straight Bismuth catalysts tend to have poor hydrolytic stability and produce spray foams with shorter shelf life.

Patcham Enhanced Bismuth Catalysts have improved hydrolytic stability and produce spray foams with longer shelf stability.

Patcham produces tin and tin-free catalysts for PU spray foams based on various blowing agents

Catalysts for CASE Urethane systems

Patcham produces a range of metal based catalysts for CASE urethane systems.

Unlike amine catalysts most metal based catalysts do not strongly promote the reaction between isocyanate and water (blow reaction, generating CO₂) and thus are less likely to create microfoam, pinholes and other surface defects.

Polyurethane CASE systems can be two component (2K) or one component (1K), both of which can be solvent-based or waterborne and may or may not require heat for curing.

Selection of catalysts depends primarily on the curing chemistry and secondly on processing requirements:

Solvent based & 100% solids 2K and 1K Urethanes	Waterborne 2K and 1K Urethanes curing:
 2K Urethane curing: Solvent evaporation followed by urethane cross-linking (gel reaction) requiring catalysts. 1K Urethane curing: Oil modified Urethanes cure by auto-oxidation – see Patcham Paint Driers for more information about catalysts (driers) for these alkyd containing coatings. 	Water soaking into the substrate or evaporating followed by cross-linking (gel reaction) requiring catalysts. May also require the application of heat. Oil modified PUDs cure by auto-oxidation – see Patcham Paint Driers for more information about catalysts (water dispersible driers) for these alkyd containing systems.
Moisture-cured (Urethane reactions initiated by water followed by gelling) or blocked isocyanates (require heat to unblock them so they can react with polyols) these systems require catalyst to accelerate curing.	
2K systems often require catalysts that can provide longer pot life (delayed action).	Require catalysts that demonstrate a degree of hydrolytic stability

Po	Polyurethane Coatings requiring urethane catalysts						
		Catalysts Requirements	Tin-based typically	Tin-free Typically			
1K	organic solvent based	Heat Cured	Fast Acting catalyst	DBTDL	Bismuth	4005, 4006, 4007	
1K	organic solvent based	Moisture Cure	Fast Acting catalyst	DBTDL			
1K	water-based	Heat Cured	Fast Acting catalyst/ Hydrolytically stable		Bismuth	4009, 4012, 4031	
2K	organic solvent based	Ambient	Delayed action	Tin mercaptides or thiogltycolates	Mix metals	4009, 9001, 19060	
2К	water-based	Ambient/ Heat cured	Fast Acting catalyst/ Hydrolytically stable		Bismuth	4009, 4012, 4031	
Other PU coatings requiring catalysts							
1K	Urethane Alkyds	Ambient/ Heat cured	Autoxidation catalyst Alkyd paint dires		Co, Zr, Ca	Alkyd Paint Driers	

PATcat					
4005	Economical				
4006	General Purpose Tine-Free				
4007	2EHA-Free				
4009	Mixed Metal				
4012	Hydrolytically Stable				
4031	Imparts improved shelf life				
9001	Concentrated Zinc-Based				
19060	Non-Toxic / Most Delayed Action				

TIN CATALYSTS

Solvent based and water based

	PATcat Tin Catalyst		
PATcat 3017	Monobutyltin trioctoate		
PATcat 3028	Dimethyltin dineodecanoate		
PATcat 3027	Dimethyltin dilauryl mercaptide		
PATcat 3030	Dimethyltin di (2-ethylhexyl thioglycolate)		
PATcat 3003	Dibutyltin diacetate		
PATcat 3004	Dibutyltin dineodecanoate		
PATcat 3001	Dibutyltin dilaurate		
PATcat 3020	Dibutyltin dilaurate (lower crystallization temperature)		
PATcat 3014	Dibutyltin lauryl mercaptide		
PATcat 3026	Dibutyltin di (2-ethylhexyl thioglycolate)		
PATcat 3046	Dibutyltin di (2-ethylhexyl thioglycolate)		
PATcat 3025	Dibutyltin di (2- ethylhexyl maleate)		
PATcat 3006	Dibutyltin acetyl acetonate		
PATcat 3018WB	Dibutyltin dilaurate		
PATcat 3031	Dibutyltin thioglyceride		
PATcat 3023	Dioctyltin diacetate		
PATcat 3024	Dioctyltin dineodecanoate		
PATcat 3005	Dioctyltin dilaurate		
PATcat 3022	Dioctyltin di (2-ethylhexyl thioglycolate)		
PATcat 3029	Dioctyltin di (lauryl mercaptide)		
PATcat 3016	Dioctyltin acetyl acetonate		

PATOX 1

• MEKO Methyl Ethyl Ketoxime

TIN-FREE CATALYSTS

Solvent based

Water based

Tin-free Catalysts					
Bismuth		Bismuth			
PATcat 4005	All purpose	PATcat 4012	Hydrolytically stable		
PATcat 4006	Most economical	PATcat 4013	Hydrolytically stable		
PATcat 4007	2EHA-free	PATcat 4007	All purpose		
Bi/Zn		Bi/Zn			
PATcat 4009	Balanced	PATcat 4009	Balanced		
Zinc		Zinc			
PATcat 9001	Most economical	PATcat 9001	Most economical		
PATcat 9002	All purpose	PATcat 9003	2EHA-free		
PATcat 9003	2EHA-free	PATcat 9009	Longer pot life		
PATcat 9009	Longer pot life				
Aluminum					
PATcat 17002					
Other Delayed action catalysts		Other Delayed action catalysts			
PATcat 19060	Better pot life, non toxic	PATcat 19060	Better pot life, non toxic		

1K Isocyanate blocking agent

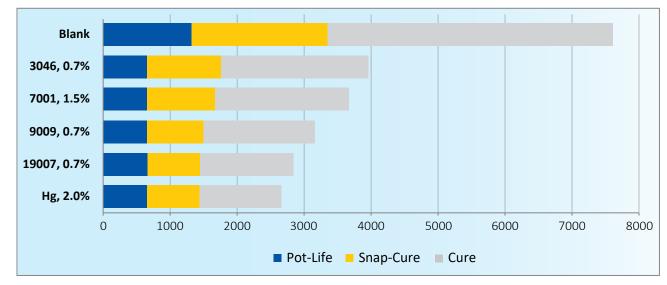
Also referred as Mercury Replacement Catalysts

- These catalysts show low initial activity at ambient temperature.
- Their activity increases as the exotherm rises over time and/or when external heat is applied.

Delayed action catalysts

PATcat					
PRODUCT					
3022	22 Tin based				
3029	Tin based				
3026	Tin based				
3046	Tin based				
7001	Nickel based				
9009 Tin-Free / Nickel-Free					
19007	Improved Snap-Cure. Colorless				

Comparison of PATcat Catalysts



Time / secs



PATCHAM (FZC)

P. O. Box : 7753, SAIF Zone, Sharjah, UAE Tel.: +971 65570035 Fax: +971 65570038 Email: patcham@eim.ae



www.patchamltd.com

PATCHAM INDIA

B-52, Pravasi Industrial Estate, Vishweshwar Nagar, Off Aarey Road, Goregoan (E) Mumbai-400 063 Tel.: +91 96191 50550

PATCHAM USA LLC

10 Commerce Road Fairfield, New Jersey - 07004 Tel.: (201) 293 4282 Fax: (201) 820 0818 Email: officeadmin@patchamusa.com

PATCHAM EUROPE BV

Dorpsstraat 24 A, 7451 BV Holten, Netherlands Tel.: +31 630723609 Emai: eu@patcham.com



The information given in this booklet is intended for technical guidance without obligation.

Ver. 2.3