PATCHAM

Patcham is a global producer of Metal-based Catalysts and Performance Additives for Paints, Coatings, Plastics and the oil industry

METAL-BASED CATALYSTS FOR POLYURETHANES AND POLYISOCYANURATES

Metal-based Catalysts for Polyurethanes (PU) and Polyisocyanurates (PIR)

General Information

POLYURETHANE INDUSTRY							
Foam			CASE				Others
Insulation		Cushioning	Coatings	Adhesives	Sealants	Elastomers MUE's	
Rigid	Spray	Flexible					

There are a few chemical reactions that occur in the formation of Polyurethane (PU) and Polyisocyanurate (PIR) to produce an array of Polyurethane products and catalysts are required:

Blow Reaction

Usually the initiating reaction.
Produces CO_2 gas often utilized in foams.

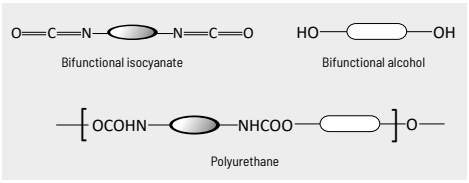
Gel reaction

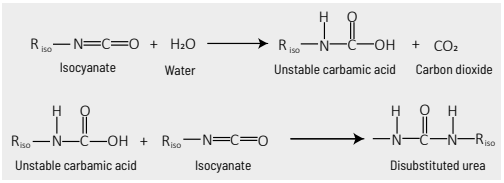
This is the chemical urethane formation reaction.

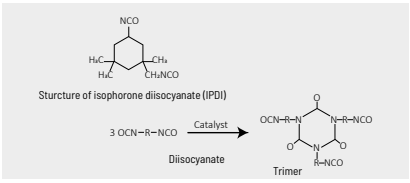
Trimerization

This is an isocyanate polymerization reaction required for production of PIR.

Reaction	
NCO/H_2O Iscoyanate / Water	**BLOW REACTION**
NCO/OH Iscoyanate / polyol	Urethane **GEL REACTION**
NCO/NCO Iscoyanate / Iscoyanate	Polymerization **TRIMERIZATION**







These reactions occur readily at temperatures above 110°C. However, at ambient temperature, without a catalyst, they are usually too slow.

Catalysts tend to catalyze several of these reactions at once, although to differing degrees. A mix of catalysts is often required to achieve a critical balance between these reactions for the desired processing and end-product properties.
Catalysts are usually designated according to the reaction they have the most influence upon.

Polyurethane and Polyisocyanurate catalysts fall into two categories:

Tertiary Amines and Metal-based Catalysts

	Tertiary Amines	Metal-based Catalysts
BLOW REACTION	**Strong**	**Weak**
GEL REACTION	**Strong**	**Strong**
Polymerization **TRIMERIZATION**	**Strong**	**Strong**

Sustainability is a consideration in catalyst selection.

Many Tertiary Amines have one or more of these detriments:

- Bad smell
- Corrosive
- VOC • Toxicity issues
- Instability with acid treated pigments
- Deactivation of HFO blowing agents
- Low Flash Point • End product discoloration

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.

Tin-Based Catalysts

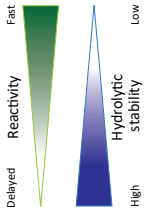
Tin containing catalysts are utilized in the production of several polymers, including Polyurethanes.

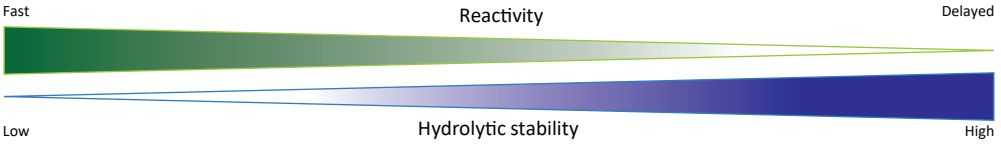
Dibutyl Tin		Metal content
PATcat 3003	Dibutyltin diacetate	33.0%
PATcat 3004	Dibutyltin dineodecanoate	20.0%
PATcat 3001	Dibutyltin dilaurate	18.0%
PATcat 3020	Dibutyltin dilaurate (lower crystallization temperature)	18.0%
PATcat 3018WB	Dibutyltin dilaurate	1.8%
PATcat 3014	Dibutyltin lauryl mercaptide	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 3031	Dibutyltin thioglyceride	26.5%

Monobutyl Tin		Metal content
PATcat 3017	Monobutyltin trioctoate	19.0%
Dimethyl Tin		
PATcat 3028	Dimethyltin dineodecanoate	23.5%
PATcat 3027	Dimethyltin dilauryl mercaptide	20.5%
PATcat 3030	Dimethyltin di (2-ethylhexyl thioglycolate)	19.0%
Dioctyl Tin		
PATcat 3024	Dioctyltin dineodecanoate	17.0%
PATcat 3005	Dioctyltin dilaurate	16.0%
PATcat 3022	Dioctyltin di (2-ethylhexyl thioglycolate)	15.0%
PATcat 3023	Dioctyltin diacetate	26.0%
PATcat 3029	Dioctyltin di (lauryl mercaptide)	15.5%
PATcat 3016	Dioctyltin acetyl acetonate	21.0%

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

PATcat		Di-acetate	Octoate	Di-neodecanoate	Di -(2-ethylhexyl maleate)	Di-laurate	Pentane dionate	Di-(lauryl mercaptide)	Di-(2 ethylhexyl thioglycolate)	Thioglyceride
Tin +4	Mono butyl		3017							
	Dimethyl			3028				3027	3030	
	Dibutyl	3003		3004	3025	3001/3020	3006	3014	3026/3046	3031
	Dioctyl	3023		3024		3005	3016	3029	3022	





Generally Tin catalysts that demonstrate a degree of delayed action tend to also demonstrate better hydrolytic stability.
Several Tin catalysts have freezing points >5C which creates a handling concern.
Tin catalyst on the whole show evidence of toxicity.

Standard Tin-free Catalysts

PATcat Standard Bismuth Catalysts		Metal content
PATcat 4007	Bismuth Neodecanoate	20.0%
PATcat 4001	Bismuth Neodecanoate	16.5%
PATcat 4036	Bismuth Neodecanoate	3.6%
PATcat 4005	Bismuth Octoate	24.0%
PATcat 4006	Bismuth Octoate	28.0%
PATcat 4016	Bismuth Neodecanoate Zinc Neodecanoate	8.0% 8.0%

PATcat Enhanced Bismuth Catalysts	
Improved hydrolytic Stability	
	Typical dosage based on polyol
PATcat 4009	**1.00%**
PATcat 4012	**0.50%**
PATcat 4020	**0.75%**
PATcat 4031	**1.50%**

PATcat Zinc Catalysts		Metal content
PATcat 9003	Zinc Neodecanoate	19.0%
PATcat 9001	Zinc Octoate	23.0%
PATcat 9002	Zinc Octoate	18.0%
PATcat 9005	Zinc Octoate	20.0%
PATcat 9009	Zinc Acetylacetonate	2.0%

Bismuth catalysts are fast acting and also tend to require higher dosage compared to Tin catalysts. Zinc catalysts tend to demonstrate a slight delay in the gel reaction compared to Tin and Bismuth.

PIR/PU Polyisocyanurate Rigid Foam

Isocyanate polymerization, particularly Trimerization, is essential in this class of polyurethanes.

Trimerization is normally the slowest of the isocyanate reactions and requires catalysts to increase the rate of production and yield of trimerized material:

PATcat 5000 series Potassium based trimerization catalysts can be used as the sole catalyst in PIR/PU systems.

	Rigid Foam PIR/PU
Blow	✓
Gel	✓✓✓✓
Trimerization	✓✓✓✓

Variations in system formulations and production equipment place different demands on the catalyst such as viscosity, OH value 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
Potassium	Octoate	DEG	15.0	5.0% max	525	3500	5001
			15.0	3.5% max	460	7000	5003
			10.0	2.0% - 4.0%	700	1200	5011
		MEG	15.3	3.0% - 4.0%	660	3500	5016
			15.0	9.5% - 10.5%	965	550	5012
	Acetate	DEG	15.0	5.5% max	910	350	5005
			13.2	2.0% max	815	350	5008
			10.0	5.5% max	1060	150	5004
		MEG	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

Special and Hybrid Potassium Trimerization Catalysts

2 Ethyl hexanoic acid (2EHA) contains 8 carbon atoms and it salts/soaps are called Octoates but it is categorized for reproductive toxicity

Contains bio renewable and low toxicity ingredients

	2-EHA-free	Smooth rise profile	Delayed Action	Sustainable
PATcat 5201	★	★		
PATcat 5021		★		
PATcat 5106	★	★	★	
PATcat 5310	★	★		★

More consistent foam product

Better for molded products

Catalysts for Soft and High resilience Polyurethane Foams

Soft foams are predominantly water blown and require strong blow reaction catalysts.

A balance is required between the blow and gel reaction to minimize foam defects.

Patcham provides tertiary amine-free and tin-free catalyst options.

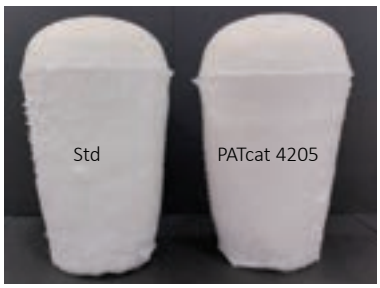
	Soft Foam
Blow	✓✓✓✓
Gel	✓✓✓✓
Trimerization	

Most soft and high resilience foams are made with combinations of tertiary amines and stannous octoate in a One-Shot process. **Tertiary Amines and Stannous Octoate, although quite effective, are poor options for sustainability as well as ease of use.**

Tin-free Stannous Octoate replacement PATcat 4205

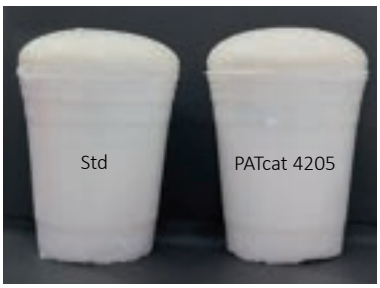
PU Foam 2lbs/ft3 30kg/m3

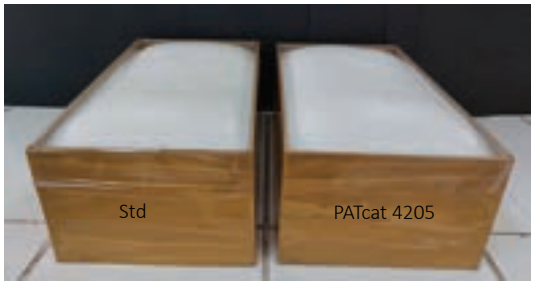
	Std	PATcat 4205
Polyether Polyol, 3000 MW	100.00	100.00
Dabco 33LV, Blow amine	0.30	0.30
Silicon surfactant	1.10	1.10
Water	4.50	4.50
Stannous Octoate	0.20	
PATcat 4205		0.40
TDI (at Index 114)	59	59
Cream time (sec)	18	17
Top of the cup (sec)	67	69
Rise time (sec)	123	125
Foam height (cm)	16	16
Density (kg/m³)	30	30

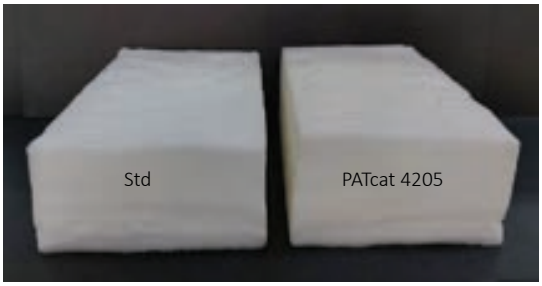


HR Foam

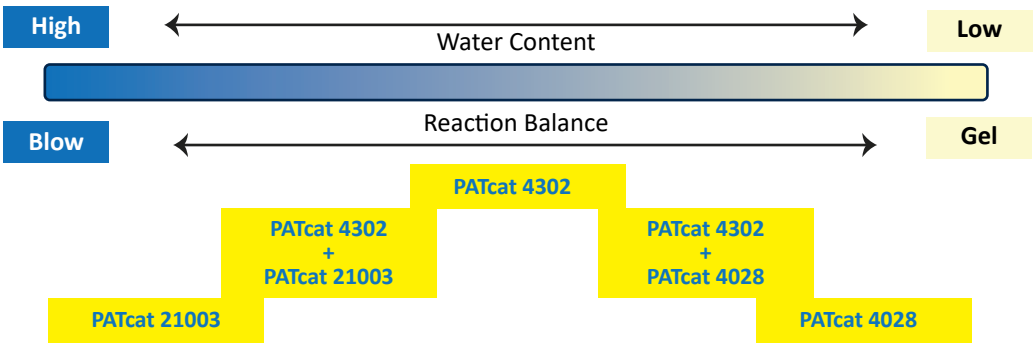
	Std	PATcat 4205
Polyol for HR foam	100.00	100.00
Water	2.77	2.77
Crosslinker	2.90	2.90
Surfactant	1.10	1.10
Teritary amine catalyst	0.12	0.12
Stannous Octoate	0.04	
PATcat 4205		0.08
TDI (at Index 105)	33	33
Cream time (sec)	21	21
Top of the cup (sec)	88	82
Rise time (sec)	170	155
Foam height (cm)	14	14.9
Density (kg/m³)	50	50







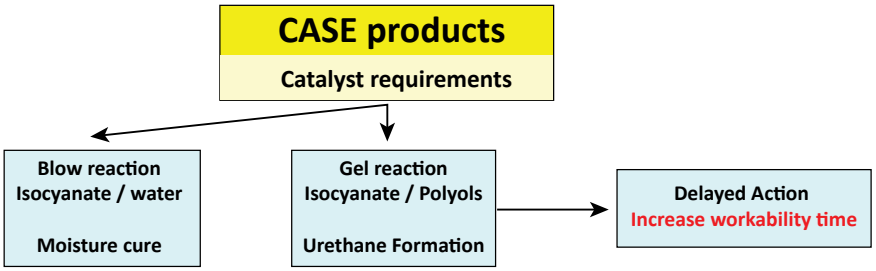
Tin-free, Amine-free Catalysts for Soft Foam and HR Foam



For low density foams with minimum defects an optimal balance is required between the Blow and Gel reactions.

Tin-free catalysts for Spray Foams

	Used in conjunction with tertiary amine blow catalysts			
	Bismuth	Bismuth / zinc	Hydrolytically stable Bismuth	Tin-free / Amine free
PATcat	4017	4009	4012	4302 21003 4028



Polyurethane

Coatings
Adhesives
Sealants
Elastomers

Coatings, adhesives and sealants

There are a variety of urethane and hybrid urethane coatings, adhesives and sealants most of which require catalysts for either production of resin intermediates or the final curing process.

ASTM Classification

	Type I Urethane Alkyd Oil modified Urethane	Type II Moisture cured	Type III Heat Cured Blocked	Type IV Catalyzed	Type V Polyol	Type VI Non-reactive
Description	1K Pre-reacted isocyanate Drying oils	1K Isocyanate terminated urethane	1K Blocked isocyanate	2K Isocyanate/polyol Cross-linking Catalyst	2K Isocyanate Polyol	1K Pre-reacted urethane
Main curing mechanism	Solvent evaporation. Oxidation of drying oil.	Atmospheric moisture initiated.	Thermal release of blocking agent. Urethane reaction.	Reaction initiated by Cross-linker.	Urethane reaction.	Solvent evaporation.
Catalyst	Alkyd paint driers	PU Catalysts	None	Reactive Diamine crosslinker/catalyst	PU Catalysts	None

Alkyd paint driers
Patcham, PATcom, PATox

PREPOLYMER production	Urea Linkage	Urethane Linkage
Tin based Catalysts		Tin based Catalysts
PATcat 3000 series		**PATcat 3000 series**
Tin-Free amine-free	Tin-Free amine-free	Tin-Free amine-free
PATcat 4017 **PATcat 4009** **PATcat 19080**	**PATcat 21003**	**PATcat 4302** **PATcat 4028**

Tin based Catalysts	Tin-Free amine-free
PATcat 3000 series	**PATcat 4017** **PATcat 4009** **PATcat 4012** **PATcat 9001** **PATcat 19080**
	Longer pot life

PREPOLYMER production	
Tin based Catalysts	
PATcat 3000 series	
Tin-Free amine-free	
PATcat 4017 **PATcat 4009** **PATcat 19080**	**Longer pot life**

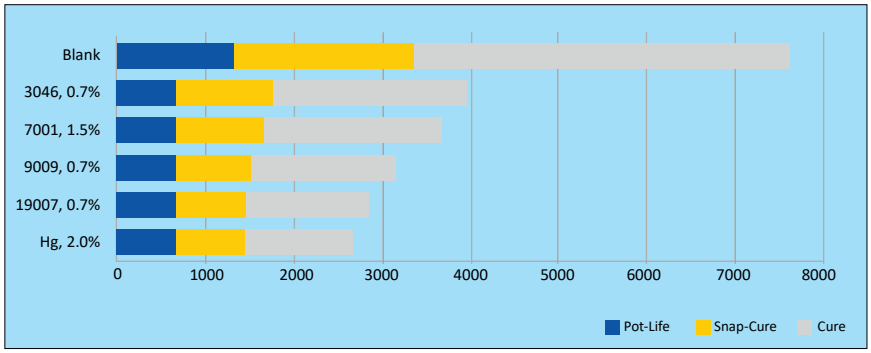
Elastomers are 2K Polyurethane systems. The polyol component is mixed with the isocyanate component just prior to application.

				Tin based Catalysts	Tin-Free amine-free
Catalysts for Elastomers	Blow / Gel	For density reduction	Used with amines	**PATcat 3000 series**	**PATcat 4017** **PATcat 4009** **PATcat 9001**
			Amines eliminated		**PATcat 4302** **PATcat 4028**
	Delayed action Gel	For increased Pot-Life	Amines eliminated	**PATcat 3000 series**	**PATcat 7001** **PATcat 9009** **PATcat 19007**

Comparison of Delayed action gel catalysts

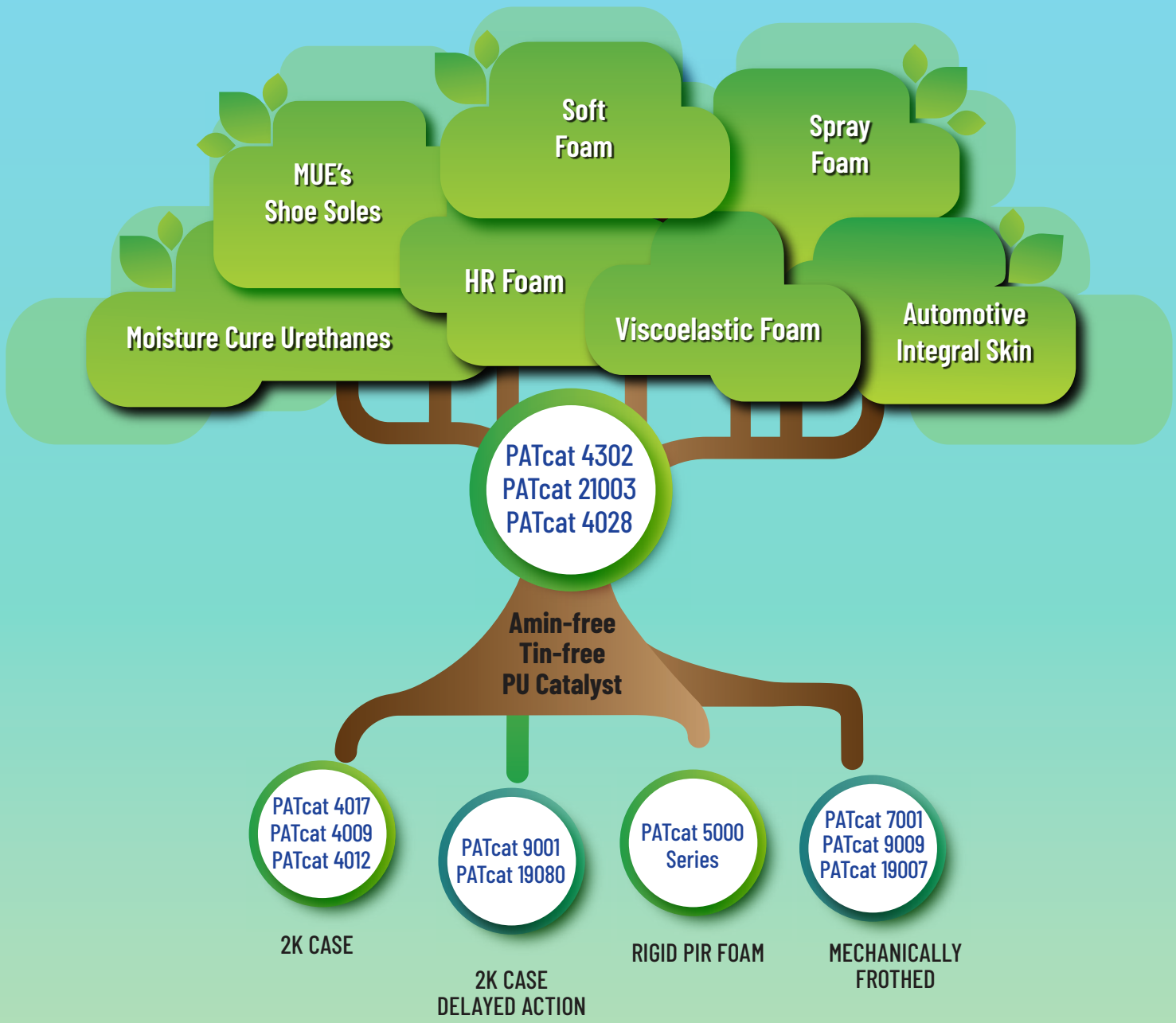
These are often requested as “Mercury Replacement catalysts.

Hg (Mercury) is included for reference only.



Like a breath of fresh air for the Urethane Industry.

Amine and Tin-free Catalysts for Urethanes



Urethane systems can be formulated without using Tertiary amine or tin catalysts.

Patcham produces a line of Tertiary Amine-free Tin-free catalysts that can balance the Blow, Gel and Trimerization reactions required to produce Urethanes Systems

Terminate dependance upon smelly, toxic, VOC Polyurethane catalysts

PATCHAM

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