VESTANAT®

BUILDING BLOCKS FOR POLYURETHANE RESINS & ELASTOMERS

vestanat® | vestanat® eCO

GO WITH THE ORIGINAL.

EVONIK
Leading Beyond Chemistry

OUR VISION

CROSSLINKERS IS THE **BEST PARTNER** FOR A **SUCCESSFUL** AND **SUSTAINABLE FUTURE**, PROVIDING **PIONEERING TECHNOLOGY** AND **GLOBAL REACH.**

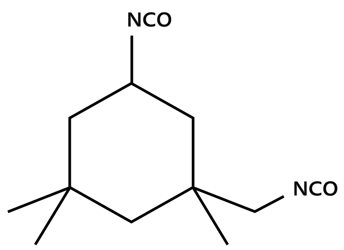
ABOUT US

PIONEER IN ISOPHORONE CHEMISTRY

Since inventing isophorone chemistry during our search for new ways to recycle and reuse acetone, Evonik's Crosslinkers business line has continued to develop high-performance isophorone-based products that improve our customers' applications.

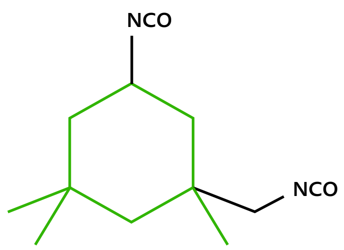
For over 60 years we've been your reliable partner and solution provider. With our global production sites we are uniquely placed to meet your local market demands.
Now, following another important breakthrough we've boosted our broad portfolio of VESTA products with our new reduced emission eCO series for more sustainable solvents, composites and coatings.

TO HELP YOU ADDRESS TODAY'S MARKET AND ENVIRONMENTAL CHALLENGES CHOOSE THE SOLUTION THAT BEST MEETS YOUR PERFORMANCE AND SUSTAINABILITY GOALS.



vestanat®

The **classical VESTA grades** are based on **virgin fossil raw materials**



vestanat® eCO

The **eCO series** is based on **renewable raw materials**

CONTENTS

1. ALIPHATIC AND CYCLOALIPHATIC DIISOCYANATES

Aliphatic and cycloaliphatic diisocyanates are specialty, reactive building blocks and serve as raw materials for numerous high-performance applications in the field of polyurethane chemistry. Compared to corresponding aromatic diisocyanates, products manufactured from (cyclo-) aliphatic diisocyanates are distinguished particularly by their high light stability and weathering resistance.

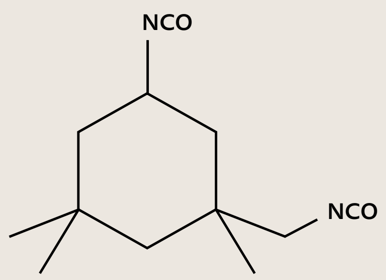
1.1 VESTANAT® IPDI

VESTANAT® IPDI (isophorone diisocyanate) is a cycloaliphatic diisocyanate and characterized by its two reactive isocyanate groups comprising differences in reactivity (primary and secondary NCO groups). This leads to a high selectivity in the reaction with hydroxyl groups bearing compounds. This unique property is advantageous for the processing of low viscosity prepolymers leading to a comparably low content of residual, monomeric diisocyanate at the same time. By choice of an appropriate catalyst (i.e. dibutyl tin dilaurate, DBTDL), the rate of conversion is increased, but also the degree of selectivity is further enhanced.
The low viscosity of IPDI-based prepolymers allows for the reduction of solvents (VOC). The methyl groups attached to the cyclohexane ring make VESTANAT® IPDI and the corresponding derivatives widely compatible with resins and solvents.

The cycloaliphatic ring itself gives products based on VESTANAT® IPDI more rigidity and a high glass transition temperature.
VESTANAT® IPDI is a colorless, low viscosity liquid with a solidification point of – 60°C. Semi-finished products, e.g. NCO terminated prepolymers have low tendencies to crystallize but rather stay liquid and are easy processable. As a cycloaliphatic diisocyanate, VESTANAT® IPDI meets all requirements for the manufacture of light stable and weatherable polyurethanes also comprising excellent mechanical properties and chemical resistance.

For more information regarding selectivity please refer to Journal of Coatings Technology, 69, 868, p. 51-57 (1997)

VESTANAT® IPDI



BENEFITS

- Differently reactive isocyanate groups
- High selectivity
- Low viscosity of prepolymers
- Low residual monomer content in prepolymers
- High glass-transition temperature
- Low tendency for crystallization
- High NCO content
- Highest toughness and flexibility at low temperature

VESTA eCO SOLUTIONS

1.1 VESTANAT® IPDI eCO

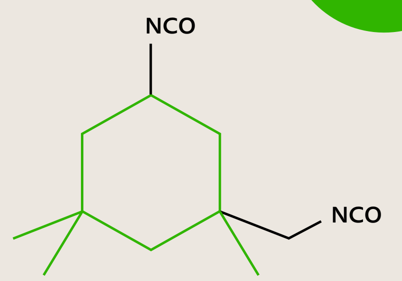
eCO stands for Evonik's aim to eliminate CO_2 through use of renewable feedstock via mass balance approach.

MASS BALANCE APPROACH
Mass balance involves mixing virgin fossil and renewable raw materials into existing systems and production processes. The renewable amount is then allocated mathematically to specific products and is certified by a neutral third party to verify the use of renewable resources across all stages of production. Mass balance is a way to keep track of the renewable quantities throughout the process and to allocate them to specific products. It allows for large-scale production and enables cost-effective solutions that meet more stingent environmental and sustainability targets.

Mass Balance allows for instant CO_2 reduction in existing plants. Giving green drop-in solutions to our customers at the best possible price.

VESTANAT® IPDI eCO

75% RENEWABLE CARBON MASS BALANCE



BENEFITS

- Same properties and performance as IPDI but with a lower CO_2 profile
- Drop-in solution
- No compromise
- ISCC-certified

1. ALIPHATIC AND CYCLOALIPHATIC DIISOCYANATES

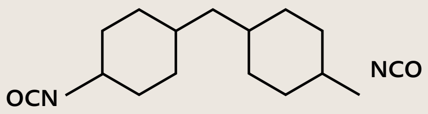
1.2 VESTANAT® H_{12}MDI

VESTANAT® H_{12}MDI (main component: dicyclyhexylmethane-4,4′-diisocyanate) is a cycloaliphatic diisocyanate with two cyclohexane rings. It resembles the hydrogenated analogue to MDI (methylendiphenylisocyanate). Nevertheless, properties of VESTANAT® H_{12}MDI differ a lot from the aromatic MDI.
VESTANAT® H_{12}MDI comprises two reactive isocyanate groups, both of secondary nature, showing nearly no differences in reactivity or pronounced selectivity. Due to this, semi-finished products, e.g. NCO terminated prepolymers show a broader molecular weight distribution resulting in an increased content of residual monomeric diisocyanate compared to VESTANAT® IPDI. Also, the viscosity of above mentioned products is significantly higher compared to similar products based on VESTANAT® IPDI.

VESTANAT® H_{12}MDI leads to superior properties of finished products, i.e. outstanding resistance against aqueous media. Also the mechanical properties are on a high level, as well as abrasion resistance and solvent or chemical resistance. Due to the aliphatic nature of the diisocyanate, the produced elastomers or coatings benefit from an excellent light stability and weathering resistance.
To combine the advantages of high selectivity and low viscosity of IPDI-based prepolymers with high resistance of H_{12}MDI-based prepolymers, VESTANAT® IPDI and VESTANAT® H_{12}MDI can also be employed as a blend. The main applications of H_{12}MDI are PUDs as well as TPUs, where high softening temperatures can be achieved.

VESTANAT® H_{12}MDI is a colorless, low viscosity liquid but tends to crystallize at temperatures below 25°C. Therefore the recommended storage temperature is about 30°C. Colder storage conditions do not harm the product, but make heating respectively a liquefying and homogenization step necessary.

VESTANAT® H_{12}MDI
Main isomer



BENEFITS

- Crystallinity/hard segment orientation
- Good chemical resistance
- Good mechanical properties
- High glass-transition temperature

1.3 VESTANAT® TMDI

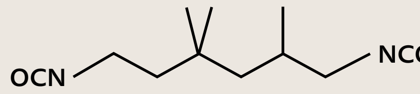
VESTANAT® TMDI (trimethyl-hexamethylene diisocyanate) is a linear, aliphatic diisocyanate, also derived from the isophorone chemistry. Structural similarities to the hexamethylene diisocyanate (HDI) are obvious but due to the three methyl groups along the chain, the products, as well as the properties of (semi-) finished products, differ signifcantly compared to HDI.

Semi-finished products, e.g. NCO terminated prepolymers based on HDI, tend to crystalize due to the pure linear structure of the diisocyanate. Using VESTANAT® TMDI instead prevents the prepolymer from crystallization. VESTANAT® TMDI also shows a good compatibility with solvents and other raw materials used in polyurethane chemistry.

VESTANAT® TMDI comprises two primary reactive isocyanate groups offering a higher reactivity compared to VESTANAT® IPDI or VESTANAT® H_{12}MDI. The similar structural surrounding is for both NCO functions leads to a low selectivity towards hydroxyl groups, but by choice of the right catalyst, the selectivity may be increased.

The linear structure, and thus the lack of cyclic structures, of the VESTANAT® TMDI leads to comparably low viscosities of semi-finished products and a pronounced flexibility to the resulting polyurethanes. These properties are especially favorable for the production of UV curing resins. With the features of low viscosity and high flexibility make the VESTANAT® TMDI also an ideal combination partner for VESTANAT® IPDI or VESTANAT® H_{12}MDI. Similar to other (cyclo-) aliphatic diisocyanates VESTANAT® TMDI offers high light stability and excellent weatherability.

VESTANAT® TMDI



Mixture of 2,2,4 and 2,4,4-Trimethyl-Isomers

BENEFITS

- Linear structure
- High flexibility
- Low tendency to crystallization
- Good compatibility
- Low glass-transition temperature

1. ALIPHATIC AND CYCLOALIPHATIC DIISOCYANATES

Main properties of (cyclo-) aliphatic diisocyanates

	VESTANAT® IPDI / IPDI eCO	VESTANAT® H_{12}MDI	VESTANAT® TMDI	Hexamethylene diisocyanate (HDI)
Molecular weight	222	262	210	168
Purity / %	≥ 99.5	≥ 99.5	≥ 99.5	- [3]
NCO content / %	37.5 – 37.8	31.8 - 32.0	39.7 – 40.0	theoretically ~ 50.0 [3]
Viscosity (23°C) / mPa s	~14	~ 30	~ 8	~ 3
Color / APHA	≤ 30	≤ 30	≤ 10	- [3]
Vapour pressure (20°C) / hPa	$6.4 * 10^{-4}$	$2.1 * 10^{-5}$	$2.7 * 10^{-3}$	$1.4 * 10^{-2}$
Selectivity @ 80°C; without catalyst [1]	4.1	< 2	< 2	2
Selectivity @ 40°C; 0.025% DBTDL [1]	11.5	< 2	6	2
Tendency for crystallization [2]	no	> 50% conversion	no	> 15% conversion

[1] 1 mol diisocyanate, 1 mol n-Butanol (NCO : OH = 2 : 1), carried out in MPA (80%)
[2] 1mol diisocyanate, 2 mol n-Octanol (NCO : OH = 1 : 1)
[3] Depends on producer

Selectivity
A selectivity of 4.1 for IPDI indicates a 4.1 times higher reaction rate of the more reactive, secondary NCO-group with OH-groups compared to the less reactive, primary NCO group in a model reaction of 1 mol diisocyanate with 1 mol n-Butanol (NCO:OH 2:1). Neither H_{12}MDI nor TMDI show a similar selectivity due to the similarly reactive NCO-groups.

TENDENCY FOR CRYSTALLIZATION

While processing pure linear diisocyanates like, hexamethylene diisocyanate (HDI) with only linear polyol components, the resulting polyurethane is also of very linear structure and offers a great option for the development of hydrogen bonds between different polyurethane chains. This leads to strong physical bonds and a separation of the reacted components from the unreacted educts also recognized as a type of crystallization (phase separation). This crystallization may happen after a very few percentages of conversion, e.g. 15% in the case of the HDI and a/m model reaction or higher degree of conversions, e.g. H_{12}MDI. IPDI and TMDI comprise some branched structures that prevent the reacted product from separation/crystallization.

REACTIVITY AND CATALYSIS

Aliphatic and (cyclo-) aliphatic diisocyanates are less reactive than aromatic diisocyanates. To accelerate their reaction with hydroxyl groups bearing compounds, tertiary amines or metal catalysts may be used very effectively. At higher temperatures, catalysts may not be needed for a sufficient degree of conversion. For some production processes however, the production of polyurethane dispersions, the lower reactivity of these diisocyanates is also an advantage.
The reaction of (cyclo-) aliphatic diisocyanates with aliphatic amines is very fast, usually too fast for a proper control and difficult to apply. Therefore special application equipment is necessary.

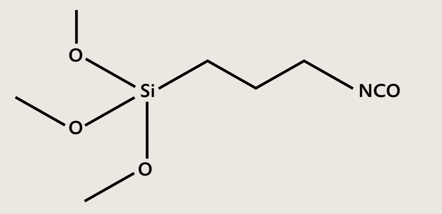
2. SPECIALTY ISOCYANATES

2.1 VESTANAT® EP- IPMS

VESTANAT® EP-IPMS is a solvent free, heterofunctional monomer, comprising both an isocyanate group and a trimethoxysilane group. With the isocyanate group, VESTANAT® EP-IPMS can be incorporated in classical polyurethane backbones. The methoxysilane groups add inorganic properties to these polymers and enhance compatibility with inorganic surfaces. Also, via hydrolysis-condenstation reaction, the methoxysilane groups can be crosslinked to polysiloxane networks introducing very high crosslink density and chemical resistance to the polymer.

VESTANAT® EP-IPMS is mainly used for the synthesis of highly resistant coatings. The polysiloxane networks incorporate glass-like substructures into the polymer matrix and induce very high hardness as well as scratch resistance while the classical PUR backbone adds the needed flexibility to the coating. The siloxane curing reaction is induced by air humidity, thus storage stable 1K formulations are possible.

VESTANAT® EP-IPMS



BENEFITS

- Links organic and inorganic substructures
- Allows moisture curing via hydrolysis-condensation
- Polysiloxane networks offer superior hardness and chemical resistance

Properties

	VESTANAT® EP-IPMS
NCO content [%]	≥ 98
Purity [%]	12.3 - 12.9
Viscosity (23°C) [mPa s]	100

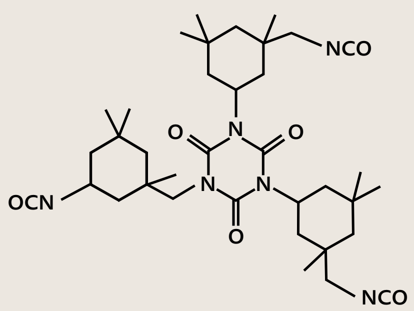
3. OTHER BUILDING BLOCKS

3.1 Solvent-free Polyisocyanates

Polyisocyanates, e.g. isocyanurate-based, are typically used as crosslinker in 2K PUR coatings. Beside this important application, these products can also be used as starting materials for blocked polyisocyanates or in resin manufacture.
Some resin technologies might have the need to impart branched structures into the polymer backbone. This can be done via the use of TMP (trimethylol propane) or other low molecular weight branched polyols. An alternative option to avoid higher viscosities compared to the use of TMP is the use of isocyanurate-based trimers. It should be noted that these products are not "trimers" in an idealized manner but also contain certain amounts of higher oligomers with higher functionality.

VESTANAT® T 1890, the polyisocyanates based on IPDI takes advantage from the (cyclo-) aliphatic ring structure and convey the high glass-transition temperature (Tg) also to coatings and elastomers. This way the resistance of coatings can be enhanced. VESTANAT® T 1890 is, as a sole product, a solid material and therefore often used dissolved in organic solvents. VESTANAT® T 1890/100 exhibits an excellent solubility in a broad range of various non-protic solvents: aromatics, esters, mineral spirit, plasticizers, acetone, MEK, etc..

Isocyanurate trimer of IPDI



BENEFITS

- Higher functionality
- High crosslinking density
- Good chemical resistance
- High Tg (VESTANAT® T 1890)

Polyisocyanate crosslinkers for 2K systems

IPDI-trimer	Solid content	NCO content	Viscosity
VESTANAT® T 1890/100	100 % (pellets)	17.3 %	solid

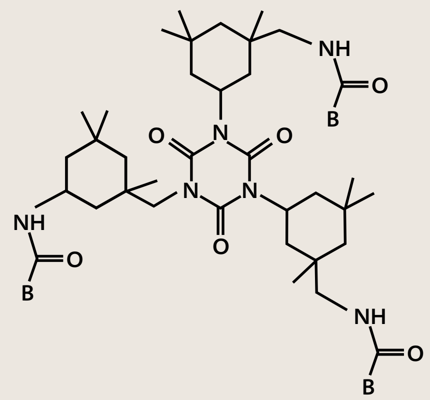
Solids content and viscosity of various solutions of VESTANAT® T 1890/100

Solvent	Solids [%]	Viscosity (23°C) [mPa s]
Acetone	75	430
MEK	75	650
Ethylacetate	75	1000
Butylacetate	70	900
Solvent naphtha	70	2000
Mineral spirit	65	2900
DINP	40	6000

3.2 Blocked Polyisocyanates

Blocked Polyisocyanates are an important alternative to melamine resins in thermosetting coating sytems for the formulation of chemical resistant high-performance coatings exhibiting excellent hardness and elasticity. VESTANAT® B 1358/100 is the perfect material to transfer this approach into waterborne thermosetting coatings due to the fact that it is supplied as a solvent-free version. This material is soluble in various types of polar solvents including, but not limited to, protic solvents, e.g. alcohols and glycols or glycolethers. Such solutions can be combined with water soluble hydroxyl - as well as carboxyl functional resins. After neutralization with tertiary amines these resin combinations can be dissolved in water by the use of suitable dispersing equipment. Also cationic versions instead of the aforementioned anionic ones are possible.
VESTANAT® B 1358/100 is well soluble in acetone. In case the acetone process is employed for the manufacture of thermosetting waterborne systems, acetone solvent can be distilled off after dispersion step.

Blocked Polyisocyanates of IPDI



BENEFITS

- High crosslinking density
- High chemical resistance
- High Tg (IPDI trimer based)
- Good solubility in organic solvents

Solids content and viscosity of various solutions of VESTANAT® B 1358/100

Solvent	Solids [%]	Viscosity (23°C) [mPa s]
Acetone	60	40
MEK	60	65
Butylacetate	60	800
Butylglycol	60	3500
Butyldiglycol	60	12200
DINP	40	20000

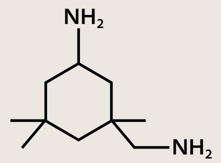
Properties

VESTANAT® B 1358/100	
Total NCO content [%]	12.3 - 12.9
Solid content [%]	100
Deblocking temperature [°C]	> 130
Melting range [°C]	115 - 130

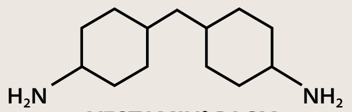
3. OTHER BUILDING BLOCKS

3.3 Diamine Chain Extenders

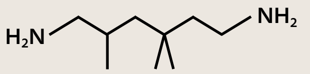
The preparation of high molecular weight polyurethane resins, e.g., polyurethane dispersions, thermoplastic polyurethanes etc. is often done in a two-step process.
In the first step an excess of monomeric diisocyanate is reacted with a di/polyfunctional OH bearing component. This is a reaction of usually moderate reactivity and various catalysts can be used to adjust reaction time and to achieve a high degree of conversion.
In the second step the build-up of the molecular weight is completed by a reaction of the NCO terminated prepolymer with short chain diols, or preferably short chain diamines to act as chain extenders. Diamines have the advantage of a high reactivity with NCO groups and this assures a fast and a complete reaction.
For the second step of the preparation of solvent-borne TPU, VESTAMIN® IPD is the preferred diamine. Alternatively, VESTAMIN® PACM or TMD can be used to suit the properties of the corresponding diisocyanates used (VESTANAT® H_{12}MDI, TMDI).



VESTAMIN® IPD eCO



VESTAMIN® PACM



VESTAMIN® TMD

vestamin® eCO

Based on renewable raw materials, **VESTAMIN® IPD eCO** makes coating systems more sustainable.
It contains 90% renewable carbon per mass balance

BENEFITS

- High reactivity
- High glass-transition temperature
- High chemical resistance

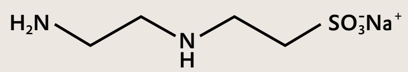
Properties

	VESTAMIN® IPD/IPD eCO	VESTAMIN® PACM	VESTAMIN® TMD
Molecular weight [g/mol]	170.3	210.3	158.3
Purity [%]	≥ 99.7	≥ 99.0	≥ 99.4
Color [APHA]	≤ 15	≤ 30	≤ 15
Water content [%]	≤ 0.2	≤ 0.1	≤ 0.2
Solidification [°C]	8	~15	-80

3.4 Chain Extender and internal Emulsifier - VESTAMIN® A 95

VESTAMIN® A 95 is a specialty building block for polyurethane dispersions (PUD) manufacturing. It combines the properties of an internal emulsifier and a chain extender.
VESTAMIN® A 95 is a ca. 50% aqueous solution of a sodium salt of an amino functional sulfonic acid. It comprises a primary and a secondary amino group. Because of the strong emulsifying power of the sulfonic group, lesser amounts of VESTAMIN® A 95, e.g. compared to dimethylolpropionic acid (DMPA), are necessary to achieve a storage stable dispersion. Similar to DMPA, VESTAMIN® A 95 is an anionic emulsifier but in contrast to DMPA, dispersions or coating formulations may also be stable at slightly acidic conditions, offering more formulation freedom.
Being a sodium salt, VESTAMIN® A 95 does not release any neutralization amines that often come along with the DMPA process. Thus, the hydrophilicity is permanent. However, due to the low content of emulsifier, chemical or hydrolytically resistance of the coating is not affected too much. As the VESTAMIN® A 95 functions as an emulsifier and chain extender at the same time, the chain extension has to be done before the actual dispersing step; the complete build-up of the molecular weight of the resin has to be done in the organic phase. Usually this requires a high amount of organic solvent. In order to avoid large quantities of co-solvent, VESTAMIN® A 95 is typically incorporated into the backbone of PUDs manufactured via the acetone process. Since high content of co-solvent is unwanted in an environmentally friendly, water-borne coating, the solvent has to be removed. Acetone can be used as an easy to remove solvent.

VESTAMIN® A 95



BENEFITS

- Internal emulsifier and chain extender
- Strong hydrophylizing power
- Stabilizing power even in neutral or slightly acidic pH range
- No release of amines

Properties

VESTAMIN® A 95	
Solid content [%]	51 ± 2
Amine value [mg KOH/g]	260 ± 20
Viscosity [mPa s]	≤ 20
Colour [Gardner]	≤ 2
pH value	11 - 12

3. OTHER BUILDING BLOCKS

3.5 Specialty Polyester - OXYESTER T 1136

As a second component for the reaction with di-/polyisocyanates mainly, OH functional components are most often used - or polyfunctional acrylates.Crosslinking of these acrylates with high Tg polyisocyanates, e.g., VESTANAT® T 1890 leads to very hard and brittle coatings. The brittleness can be easily reduced by combining the acrylate with some parts of OXYESTER T 1136.
OXYESTER T 1136 is polyester-based on only linear raw materials displaying a low viscosity without any solvents. Due to the linear structure OXYESTER T 1336 acts as a flexibilizing agent in PUR coatings or elastomers.

The low viscosity of OXYESTER T 1136 is also of advantage in the production of NCO terminated prepolymers that are used for moisture curing coatings in the construction area.

BENEFITS

- VOC-free
- Liquid
- Low viscosity
- Flexibilizing
- Low color
- Good compatibility

Properties

OXYESTER T 1136	
OH value [mg KOH/g]	107 ± 10
Viscosity [mPa s]	4000 ± 800
Molecular weight [g/mol]	~1000
Water content [%]	≤ 0.1
Solidification [°C]	~ - 20

4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.1 NCO terminated Prepolymers

Isocyanate prepolymers are important products or intermediates in polyurethane chemistry. Prepolymers are used as a "final" product in various applications in which the crosslinking is occurring after application via moisture curing. Examples are moisture curing coatings for roof and deck coatings, adhesives and sealants incl. reactive hot-melt adhesives.

On the other hand, prepolymerization of diiscocyanates, so called quasi-prepolymers, is used to adjust the viscosity profile and the ratio of both components for better mixing with the polyol component in 2K applications. NCO prepolymers are also key intermediates in PUR resin manufacture like polyurethane dispersions (PUD), urethane acrylates (UV resins), etc.
In all these cases the resin designer has various parameters to influence key properties of prepolymers like viscosity, monomer content, etc.

Moisture Curing Coatings

Printing Inks

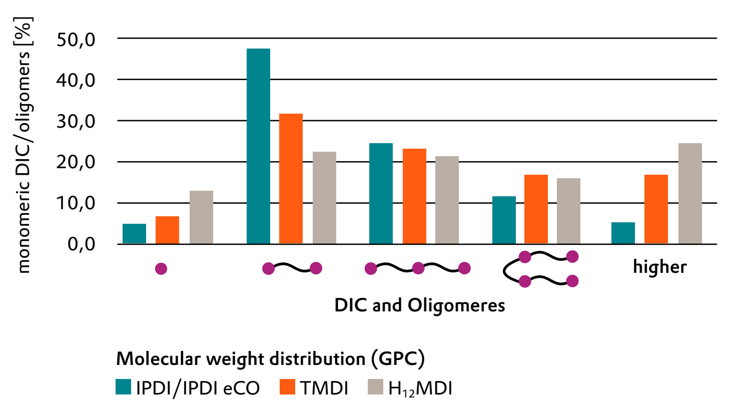
4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

Viscosity of prepolymer and content of residual, monomeric diisocyanate

VESTANAT® IPDI has two reactive isocyanate groups comprising differences in reactivity (primary and secondary NCO groups). This leads to a high selectivity in the reaction with hydroxyl groups bearing compounds. By choice of an appropriate catalyst, the rate of conversion is increased, but also the degree of selectivity is further enhanced. This means, that the more reactive NCO function reacts with the polyol component and the less reactive NCO function stays mainly unreacted. This way the less reactive group does also not push the formation of longer oligomer chains. Low content of (higher) oligomers has the advantage of lower viscosity, but even more importantly, the content of residual (unreacted) monomer content is kept very low.
Due to the high selectivity of VESTANAT® IPDI, prepolymers based hereon comprise a low content of monomeric IPDI and a low viscosity at the same time.
VESTANAT® H_{12}MDI and TMDI don't have such a high selectivity, resulting in a higher content of monomeric diisocyanate.

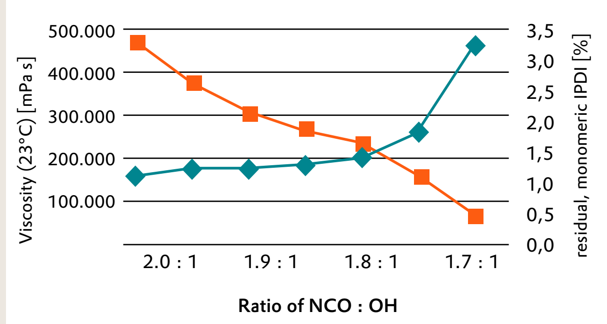
Nevertheless the viscosity of the TMDI based prepolymer is lower due to the linear structure of the molecule and the viscosity of the H_{12}MDI-based prepolymer is even higher than the IPDI alternative due to the double ring structure.
Exemplary investigation of the preparation of prepolymers based on hydroxypivalic acid NPG ester (HPN) and different diisocyanates demonstrate this aspect of low viscosity and low residual monomer content. HPN is not a typical polyol component for PUR chemistry but due to its branched structure it prevents the reaction product from crystallization even in the combination with H_{12}MDI.
The processing of the NCO terminated prepolymer took place at a NCO : OH ratio of 2 : 1, 80% in MOP-acetate, DBTDL catalysis (0.04%) at 50°C.

Monomeric diisocyanate depending on the kind of isocyanate



	IPDI/ IPDI eCO	TMDI	H_{12}MDI
NCO content [%]	10.1	10.2	9.0
monomeric DIC	6.1	9.2	14.8
Viscosity (23°C) [Pa s]	12	0.6	23

Monomeric diisocyanate depending on the stoichiometric ratio of diisocyanate and polyol component



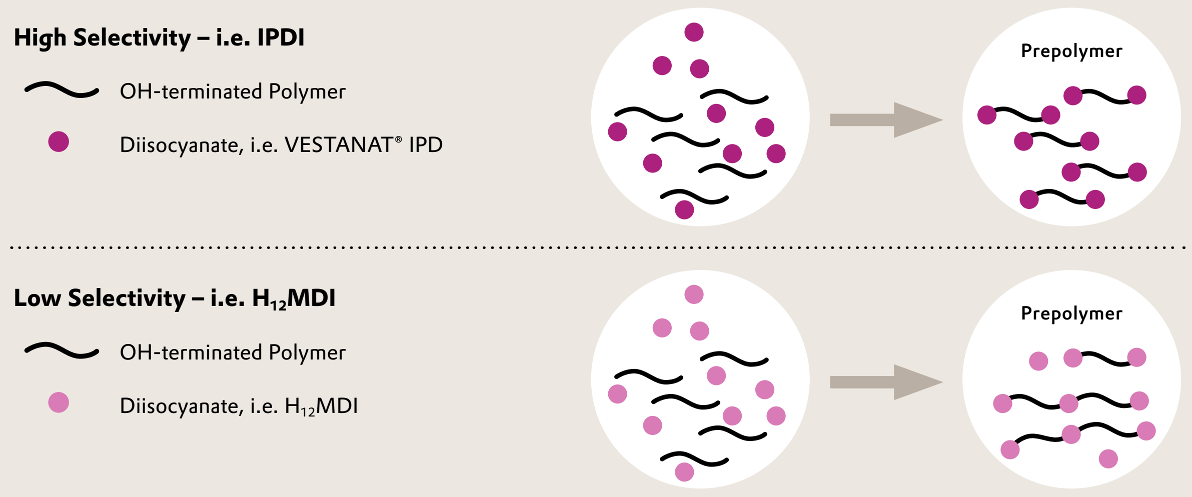
NCO terminated prepolymer based on IPDI and Oxyester T 1136 (linear, MW 1000)

monomeric IPDI

Viscosity

An option to lower the content of residual, monomeric diisocyanate in the prepolymer is to reduce the portion of the diisocyanate, to drive the ratio of NCO : OH from theoretically 2 : 1 towards, e.g., 1.7 : 1. An increase in viscosity has to be taken into account as the formation of higher oligomers can not be excluded. The main reason to achieve a low content of residual, monomeric diisocyanate is its toxicity potential and a reduction of monomeric diisocyanate leads to a reduction of the hazard.

Another option to reduce the monomeric diisocyanate in NCO terminated prepolymers is to remove the residual diisocyanate after the conversion by distillation, usually by short distance distillation. In case this distillation step is included in the processing anyway, this offers the possibility to react a higher excess of diisocyanate with the polyol component, e.g., NCO : OH = 5-10 : 1, to avoid the formation of higher oligomers ending with a lower viscosity. The distilled diisocyanate can be recycled in the process.



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.1.1 Moisture Curing Coatings

Moisture curing of NCO terminated prepolymers offers a very smart approach for a convenient application and high-performance coatings at the same time. Other than in classical 2K polyurethane systems, there is only one component that has to be applied. Air humidity induces the curing reaction by decomposing NCO groups to an amine. The amine subsequently reacts with remaining isocyanates to form polyurea bonds to high molecular weight polymers for coatings. Thus, mixing of components is not necessary, which saves one error-prone process step. This also implies that there is no pot-life that has to be taken into account.
For durable and UV resistant coatings, VESTANAT® IPDI is the isocyanate of choice. Due to its (cyclo)aliphatic ring structure, VESTAMIN® IPDI leads to an ideal balance of hardness and flexibility. Additionally, the high selectivity offers the chance for low residual monomeric IPDI in the prepolymer. This is advantageous for toxicity reasons, classification and labeling. Coatings purely based on linear prepolymers may lead to very soft coatings.

To avoid this, to increase hardness, two options are considerable:

- utilization of branched polyol components for the prepolymer processing
- combination of a linear prepolymer with polyisocyanates, especially with cycloaliphatic polyisocyanates based on IPDI, e.g. VESTANAT® T 1890 (different solvent cuts available). This way the properties of the coating can easily be adjusted.

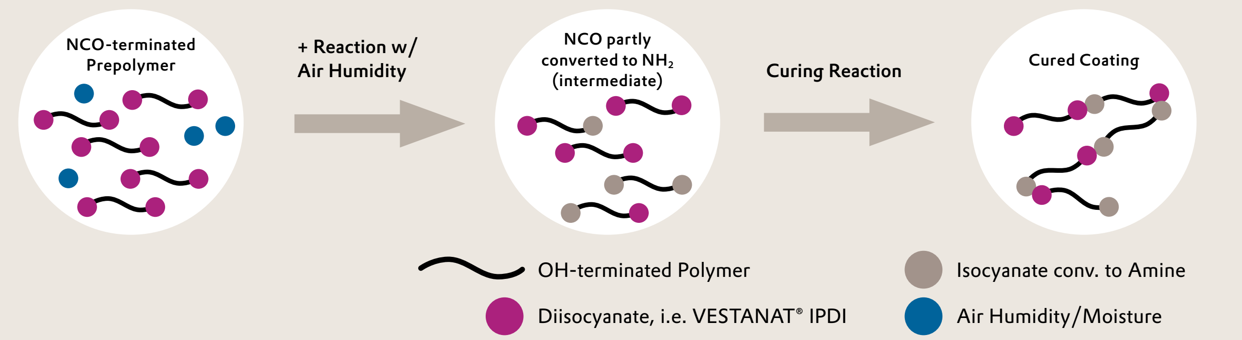
ADVANTAGES

- 1K coatings system
- Curing at ambient temperature or even lower
- Highly crosslinked coating
- Excellent adhesion and chemical resistance

General Applications
Coatings for plastic, wood, maintenance, construction (flooring)

Recommended products for moisture curing coatings

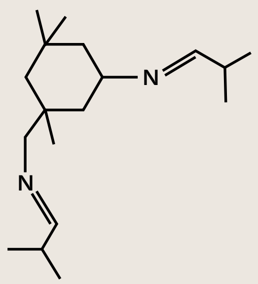
Isocyanates for resin manufacture	VESTANAT® IPDI/IPDI eCO | H_{12}MDI
Polyol component for resin manufacture	OXYESTER T 1136
Polyisocyanates	VESTANAT® T 1890
Accelerator	VESTAMIN® A 139



VESTAMIN® A 139

VESTAMIN® A 139 is a cycloaliphatic bisaldimine. VESTAMIN® A 139 decomposes under air humidity to an amine, which may react with isocyanates very fast. It is therefore used as an accelerator for moisture curing systems, curing times can be reduced significantly. However, due to a side reaction (by en/imine tautomerism) taking place over several days to a few weeks, viscosity increases during storage. So, the solution should be used as 2K approach and then has a very long pot life.
As VESTAMIN® A 139 reacts with water very fast, there is also an option to use it as a water scavenger in 2K PUR coatings to prevent the formation of gas bubbles by release of CO_2. The reaction of VESTAMIN® A 139 with water may also be beneficial when used in a 2K PUR coating. The VESTAMIN® A 139 decomposes under the influence of air humidity and splits back a highly reactive diamine. This diamine subsequently reacts with NCO functions left in the coating very quickly and thus leads to a very fast curing.

VESTAMIN® A 139



BENEFITS

- High reactivity with water
- Accelerator for moisture curing systems
- Water scavenger
- Fast curing 2K PUR

Properties

VESTAMIN® A 139	
Amine value [mg KOH/g]	400 ± 10
Purity [%]	≥ 96
Viscosity (23°C) [mPa s]	20 - 30
Colour [APHA]	≤ 150
Amine equivalent weight [g/val]	~ 140

4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.1.2 Adhesives and Sealants

Reactive hot-melt adhesives are applied in molten state. When the adhesive cools down, a physical drying process happens first, and afterwards moisture from the air causes a chemical reaction to a completely cured elastomer. This way reactive hot melts combine the application benefits of hot-melt adhesives with the bonding performance of 2K adhesives.
For reactive hot-melt adhesives, e.g. polyesters are end capped with diisocyanates also leading to an NCO terminated prepolymer.

In general, aromatic isocyanates are used in this application field. Only for glue joints to remain visible, aliphatic diisocyanates, e.g. VESTANAT® IPDI are preferred.
Moisture curing (one component) sealants are also used for in glazing for automotive applications (i.e. wind screen). As those sealants are exposed to sunlight, aliphatic isocyanates are of advantage preventing degradation.

ADVANTAGES

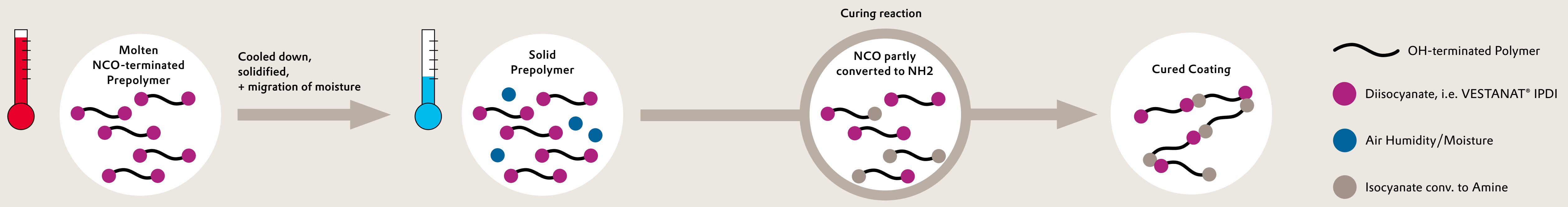
- VOC-free, 100 % solids content
- High resistance to water
- High heat resistance
- High production speeds due to short setting times
- UV resistant and light-stable in case of aliphatic diisocyanates

General Applications
Flexible packaging, Automotive glazing, Electronics

Recommended products for reactive hot melt adhesives (RHM)

Isocyanates	VESTANAT® IPDI/IPDI eCO | H_{12}MDI
Polyol component	* Dynacoll®

* For more information – please follow: www.evonik.com/dynacoll



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.2 Polyurethane Dispersions

Polyurethane dispersions (PUDs) are a class of coatings comprising polyurethane/polyurea resins dispersed in water. The final coating is achieved by physical drying. Since the main volatile component is water, PUDs are an excellent alternative to traditional solvent-borne polyurethane coatings, gaining more importance due to the increasing demand for more environmentally friendly solutions. VESTANAT® IPDI, and H_{12}MDI are the most important raw materials for manufacturing water-based polyurethane dispersions. The polyol components (molecular weight, ratio of short chain diols or higher functional components) have a big influence on the coatings properties of PUDs. Nevertheless, the diisocyanate influences these properties significantly. VESTANAT® IPDI is the major diisocyanate for PUDs due to its high selectivity leading to low prepolymer viscosities, thus offering an easy processing and excellent coating properties. If there is a demand for higher hydrolytic stability, VESTANAT® H_{12}MDI is better suited, but the higher viscosity of prepolymer or higher amount of co-solvent has to be taken into account. For very high flexibility or to adjust the flexibility of VESTANAT® H_{12}MDI based PUD for coatings on leather or textile, before mentioned diisocyanates can partially be substituted by VESTANAT® TMDI.

ADVANTAGES

- Introduction of hard segments at low prepolymer viscosity
- High flexibility also at low temperatures
- Excellent light-stability and good abrasion resistance
- Low co-solvent level or even totally VOC-free
- Optional crosslinking of PUD to enhance properties

General Applications

Leather-, Textile- and Paper coatings, Parquet coating, Industrial coatings, Printing ink binder, Glass fiber sizing, Adhesives

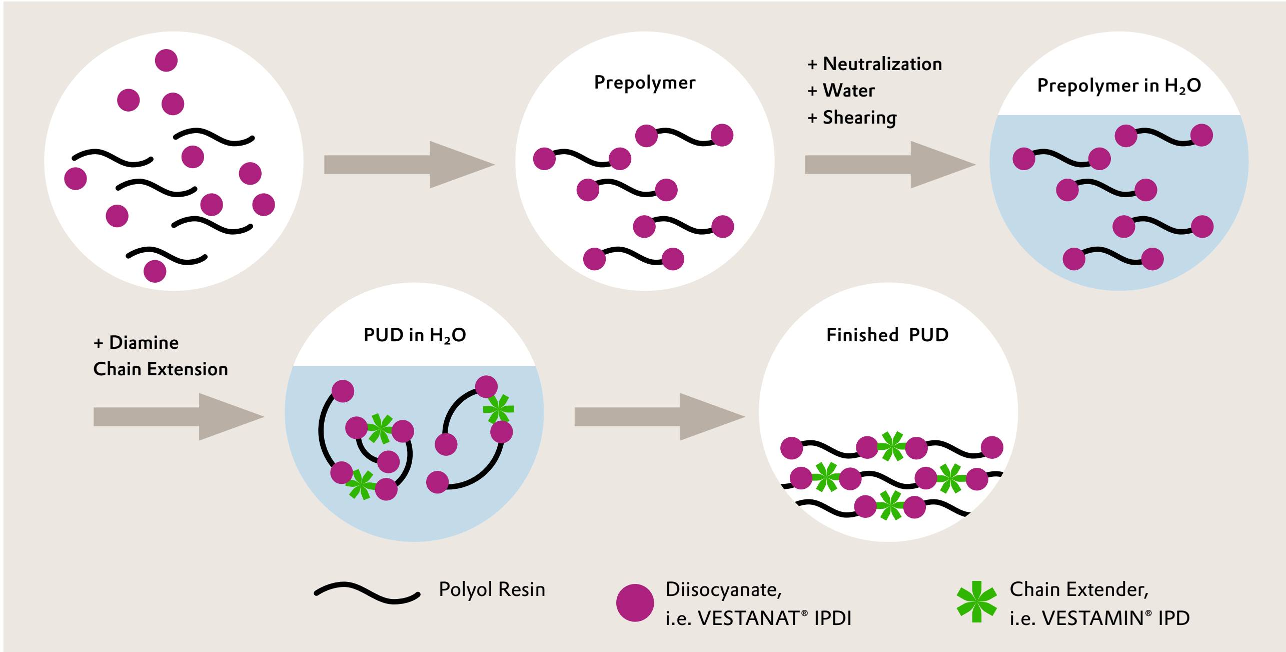
Further building blocks for PUDs

The preparation of PUDs classically involves a chain extension of the prepolymers to build-up the high molecular weight of the resin. Typically, ethylene diamine (EDA) is used for this purpose. To obtain higher or more durable gloss etc., higher molecular weight diamines that may also have cycloaliphatic structures from the VESTAMIN® product range are also used for the chain extension, as well. For speficic purposes VESTAMIN® A 95 is a highly powerful emulsifier and chain extender

Recommended products for polyurethane dispersions (PUDs)

Isocyanates	VESTANAT® IPDI/IPDI eCO | H_{12}MDI | TMDI | DC 1241 | IPMS
Blocked polyisocyanate	VESTANAT® B 1358/100
Chain extender	VESTAMIN® IPD/IPD eCO | PACM | TMD | A95
Polyol component	OXYESTER T 1136

PUD production process



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.3 Artificial Leather

As a sustainable substitute for natural leather, polyurethane (PU)-based synthetic leather already has a more environmentally friendly manufacturing process. However, current solvent-based production technology still has a negative impact on the environment.

Evonik offers a range of products that are suitable for more environmentally friendly processes and can replace traditional solvent-intensive processes. Evonik's established isophorone based solutions for aqueous polyurethane dispersions comply with the Zero Discharge of Hazardous Chemicals (ZDHC) Manufacturing Restricted Substances List (MRSL) and fulfill our commitment to sustainability with practical measures.

Our VESTANAT products are not only suitable for classic PUD applications, but also for the newly developed and patented solvent free and 100%-solid 2K or even 1K approaches.

4.3.1 Aliphatic 2K PU technology

Instead of pre-synthesizing the polymer and dispersing it in water, in this approach, resins and hardeners are applied in a mixing step directly to the substrate and cure in place in only a few minutes at moderate temperatures. A clear advantage is the process speed associated with the reaction speed.

This process is well-known from the coating industry, but also established to produce elastomers. Evonik has developed formulations based on VESTANAT® IPDI and VESTANAT® TMDI to transfer this to artificial leather manufacturing. This offers huge advantages in terms of efficiency and sustainability.

4.3.2 Aliphatic 1K PU technology

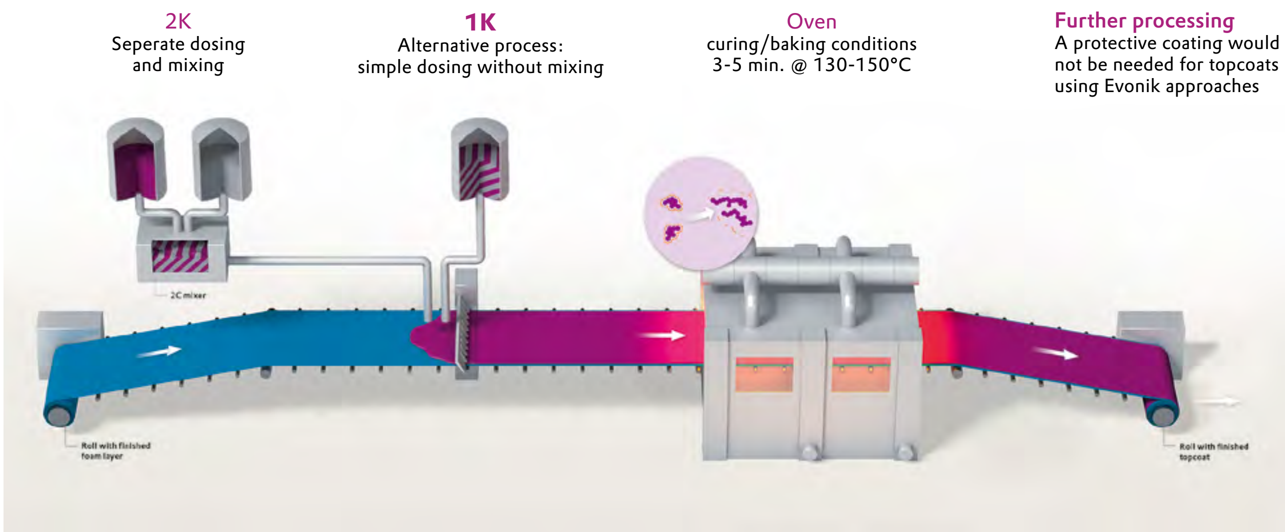
We have combined the VESTANAT® TMDI and VESTANAT® IPDI based 2K process with state-of-the-art blocking technology to offer a 1K storage stable system. The reaction partners are chemically blocked and brief heating to 130-150°C initiates the curing reaction.

With this process, the base layer and the skin layer in the artificial leather can be combined, for example, to enable particularly flexible and stretchable skins. A finish top layer only is required for very special requirements.

ADVANTAGES

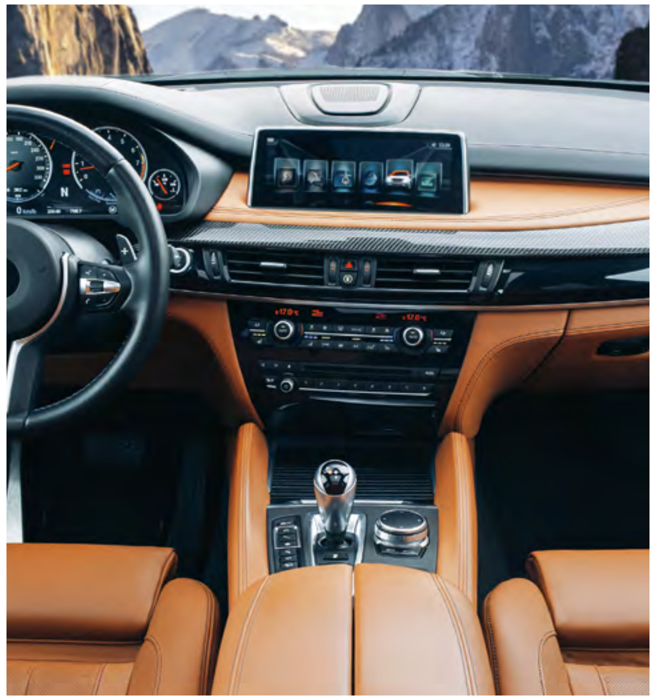
- light stability and weathering resistance
- 100% solid and solvent-free system
- fast curing and lower baking temperature to 3-5min @120-150°C
- high flexibility and mechanical performance
- convincing "touch and feel"
- Direct use of existing 1K/2K equipment for production

General Applications
Furniture, Seats, Handbags, gloves, shoes, clothing, car seats



Recommended products for Artificial Leather

Isocyanates	VESTANAT® IPDI | H_{12}MDI | TMDI
Hardeners	VESTAMIN® IPD | PACM | TMD



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.4 Radiation Curable Resins

Radiation curable resins are a solution for low-VOC coatings. Since the resins usually are liquid, viscosity can be adjusted by the use of a reactive diluent. Instead of physical drying, the solidification on the film is caused by a curing reaction induced by UV or electron beam radiation. This reaction usually takes place in seconds. As there is no need to eliminate solvents, there is no need for large drying ovens and the process is very fast, economic and environmental friendly.
Most UV curable coatings are based on acrylate functional resins. Diisocyanates like VESTANAT® IPDI, H_{12}MDI and TMDI are widely used to produce numerous oligomers to take advantage of urethane groups in the coating for high flexibility, the right softness/hardness and light-stability.
Casting resins, i.e. for dental fillings, are another application for UV-curable resins. VESTANAT® TMDI based resins have very low viscosities and are thus the preferred solution in this application. Even with high loads of fillers, the resins can be used without solvents/VOC/reactive diluents.

ADVANTAGES

- Curing within seconds by radiation, very fast process
- Low / no emission (VOC)
- Low/no solvents and also no water → no drying necessary
- Low curing temperature, so suitable for heat sensitive substrates like wood, plastics
- Low coating thickness, low material consumption
- High crosslinking, high weatherability
- High toughness, high transparency and high gloss
- Excellent scratch resistance and chemical resistance

UV-PUDs

Waterborne radiation curing technology can be seen as a combination of a polyurethane dispersion offering a solvent-free, low-viscosity resin base with additional crosslinking for outstanding performance. This can be achieved e.g. by introducing acrylate functions into the PUR backbone and/or by utilizing reactive diluents instead of conventional solvents, used in the processing of PUDs. This results in higher chemical and mechanical resistance compared to classical PUD while keeping their high flexibility.

General Applications
Hard coat for plastic films, Coating for (photo) paper, Coating of glass (e.g. eyeglasses), protection of printed circuit boards, UV curable resins for dental applications

Comparison of viscosities (23°C) of UV resins: 1 mol PTMEG (650g/mol), 2 mol diisocyanate (DIC), 2 mol hydroxyethylacrylate (HEA)

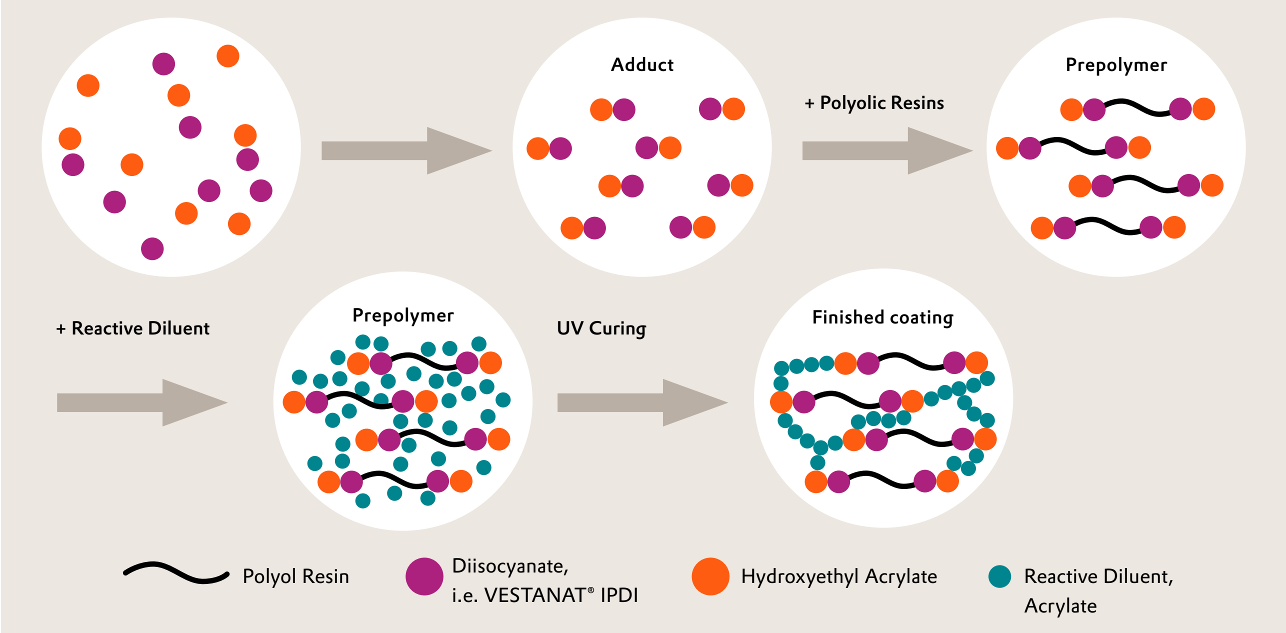
		VESTANAT® IPDI/IPDI eCO	VESTANAT® H_{12}MDI	VESTANAT® TMDI
100% resin	mPa s	430.000	1.400.000	37.500
70% in TMP-TA	mPa s	28.800	300.000	8.200
70% in HDDA	mPa s	3.900	175.000	1.800

TMP-TA = trimethylolpropane triacrylate, HDDA = hexanediol diacrylate

Recommended products for radiation curable urethane acrylates (UV resins)

Isocyanates	VESTANAT® IPDI/IPDI eCO | H_{12}MDI | TMDI | DC 1241
Polyol component	OXYESTER T 1136

UV-resin production process



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.5 Solvent-borne TPU

Similar to PUD, solvent-borne TPU are derived from NCO terminated prepolymers, which is extended to a high molecular weight resin by a reaction with mainly a diamine, e.g. VESTAMIN® IPD. To adjust the molecular weight, mono-functional amines are used as chain terminators. As these are mainly linear, high molecular weight polymers, these resins are soluble but usually need high amounts of polar solvents.

VESTANAT® IPDI is preferred in this application over VESTANAT® H_{12}MDI due to its lower viscosity. VESTANAT® H_{12}MDI may be used despite the higher viscosity to achieve higher resistance and better hydrolytic stability of the coating.

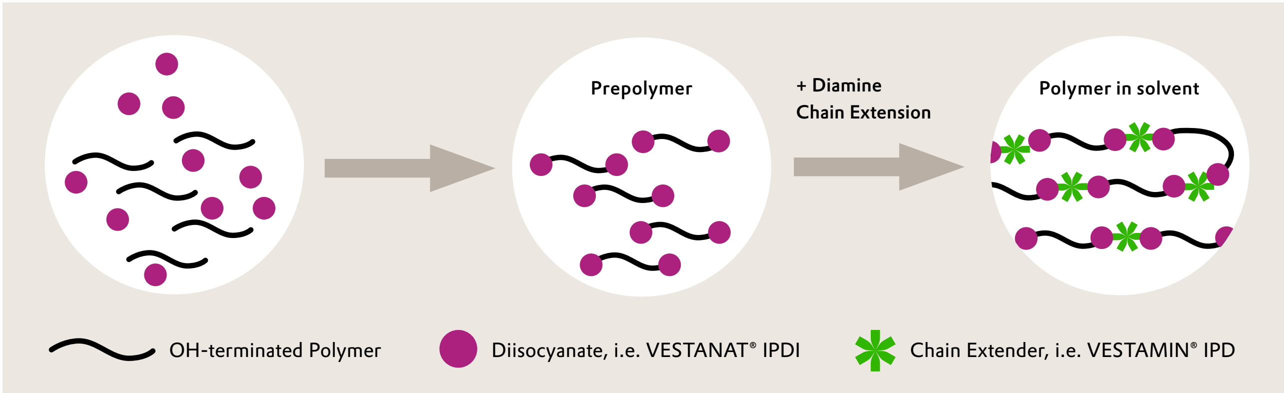
ADVANTAGES

- Pure physically drying, 1K system
- Fast drying, due to high volatile solvent
- Very flexible coatings
- Very good adhesion

General Applications
Flexible coating for genuine leather, artificial leather, textile or any other very flexible substrates. This kind of resin are also used as printing ink binder for retort food packaging or to avoid toluene as a solvent as an alternative to chlorinated polyolefine ink binders.

Recommended products for solvent-borne TPU

Isocyanates	VESTANAT® IPDI/IPDI eCO | H_{12}MDI
Chain extender	VESTAMIN® IPD/IPD eCO | PACM
Polyol component	OXYESTER T 1136



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.6 PUR Elastomers

Polyurethane elastomers are elastic, rubbery materials that have the unique property of a shape memory effect. After deformation, the material gets back to the original shape. PUR elastomers cover a broad range of hardness from as low as 10 Shore A to even more than 80 Shore D. They are tough, abrasion resistant and show high mechanical strength and resistance to most solvents and chemicals. PUR elastomers are produced by reacting isocyanates with combinations of high molecular weight polyol components and low molecular weight diols or diamines as chain extender. For non-discoloring applications, aliphatic isocyanates like VESTANAT® IPDI or VESTANAT® H_{12}MDI are chosen. Depending on the functionality of the reaction partners, the resulting elastomer may be a linear, thermoplastic PUR (TPU) or a highly crosslinked duromer.

2K Elastomers


TPU

4.6.1 Two Component Elastomers

For 2K elastomers both reaction partners are mixed just before they are applied. To adjust for a convenient or fixed/pre-defined mixing ratio, the isocyanate is used as a quasi- prepolymer, pre-reacted with some amounts of usually linear polyol components. This provides the advantage that two more comparable components, with respect to volume/mass, have to be mixed and also the increase in viscosity of the isocyanate component assures a better mixing result.
For 2K elastomers, usually raw materials, both isocyanates and polyol components, with higher functionality are used to generate a high crosslinking density leading to superior properties.

VESTANAT® T 1890/100 (IPDI based polyisocyanate) dissolved in VESTANAT® IPDI (monomeric diisocyanate) is an ideal isocyanate component for introducing high crosslinking and high Tg (glass transition temperature) hard segments. A mixing ration of IPDI polyisocyanate : monomeric IPDI = 40 : 60 leads to an easy processable viscosity of ~ 900 mPa s. As monomeric IPDI is a toxic raw material, the processing is only allowed in safe working environments.

ADVANTAGES

- Easy to make (high reactive raw materials)
- Coverage of a wide range of hardness
- High chemical resistance
- Excellent abrasion resistance
- Excellent elasticity
  - if hard, still flexible
  - if soft, not tacky
- High transparency
- Non-yellowing

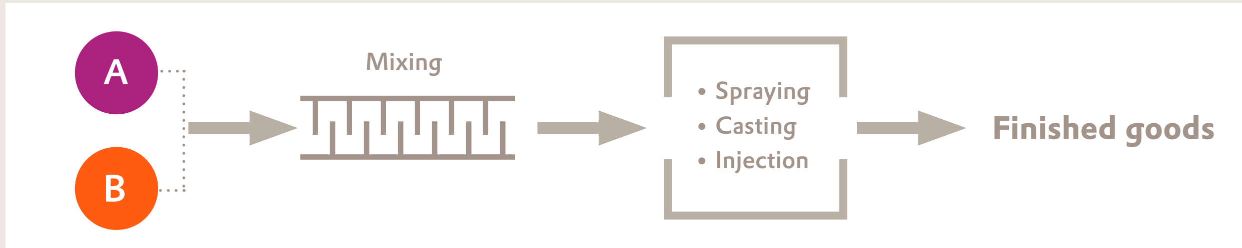
Recommended products for 2K elastomers

Isocyanates	VESTANAT® IPDI/IPDI eCO | H_{12}MDI
Polyisocyanates	VESTANAT® T 1890
Polyol component	OXYESTER T 1136

General Applications

There are some different options for processing 2K elastomers, but commonly heated reaction components are circulated to a multi component mixing head and then released to either:

- Printed paper/plastic/metal or concrete substrate
- Open mold (casting application/ spray application)
- Closed mold (resin injection molding RIM/ clear coat mold (CCM)
- Conveyer belt for a free expansion to a slab stock foam (foam application)



4. APPLICATIONS FOR (CYCLO-) ALIPHATIC DIISOCYANATES

4.6.2 TPU (Thermoplastic Polyurethane)

Different than other PUR application, TPU are fully reacted products mainly provided as granules or films. Granulated TPU can be injected or extruded like many other thermoplastic materials to produce a wide range of products. TPU films based on aliphatic isocyanates are ideal materials for laminated glass sheets, e.g. for security glazing.
For the processing of TPU by injection or extrusion, a fast solidification is of advantage. Due to its tendency for crystallization, VESTANAT® H_{12}MDI is preferred in this application.
As TPU are mainly based on linear components to provide thermoplastic properties, TPU are soluble in appropriate solvents and may also be processed already in solvent, e.g. for coating applications (solvent-borne TPU).

ADVANTAGES

- High resistance to abrasion and wear
- High impact/scratch resistance and high durability
- Rigid but also flexible at low temperature
- High flexibility without plasticizers
- High flexural strength and good rebound
- High temperature resistance and high dimension stability
- Good adhesion to various substrates
- Outstanding UV resistance and color fastness

General Applications

Footwear, Sport & leisure (ski boots, skate boot shells), Automotive interior (panels (slush molding), Various trim parts), Agriculture (animal ID tags), Films (membranes, Lamination (safety glazing), Surface protection in automotive and electronics), Profiles as light guides/strips

Recommended products for TPU

Isocyanates	VESTANAT® H_{12}MDI

5. RAW MATERIALS AND APPLICATIONS AT A GLANCE

Building blocks for polyurethane resins & elastomers

	Resins for Coatings and Adhesives				Elastomers		
	Polyurethane dispersions	Radiation curable	Solvent borne TPU	NCO terminated Prepolymers	2K Elastomers	TPU	available 1)
Monomeric Diisocyanates							
VESTANAT® IPDI/IPDI eCO	x	x	x	x	x	(x)	ww
VESTANAT® H_{12}MDI	x	x	x	(x)	x	x	ww
VESTANAT® TMDI	x	x	(x)	x	x	(x)	ww
Specialty Isocyanates							
VESTANAT® EP-DC 1241	x	x	-	-	-	-	ww
VESTANAT® EP-IPMS	(x)	-	-	-	-	-	ww
Chain extender							
VESTAMIN® IPD/IPD eCO	x	-	-	-	-	-	ww
VESTAMIN® TMD	x	-	-	-	-	-	ww
VESTAMIN® PACM	x	-	-	-	-	-	ww
Hydrophilizing Chain Extender							
VESTAMIN® A 95	x	-	-	-	-	-	ww
Blocked Polyisocyanates							
VESTANAT® B 1358/100	x	-	-	-	-	-	ww
Specialty Polyester							
Oxyester T 1136	x	x	x	x	x	(x)	ww
Other Specialties							
VESTAMIN® A 139	-	-	-	x	-	-	ww

1) ww = Worldwide; E = Europe; N = NAFTA

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