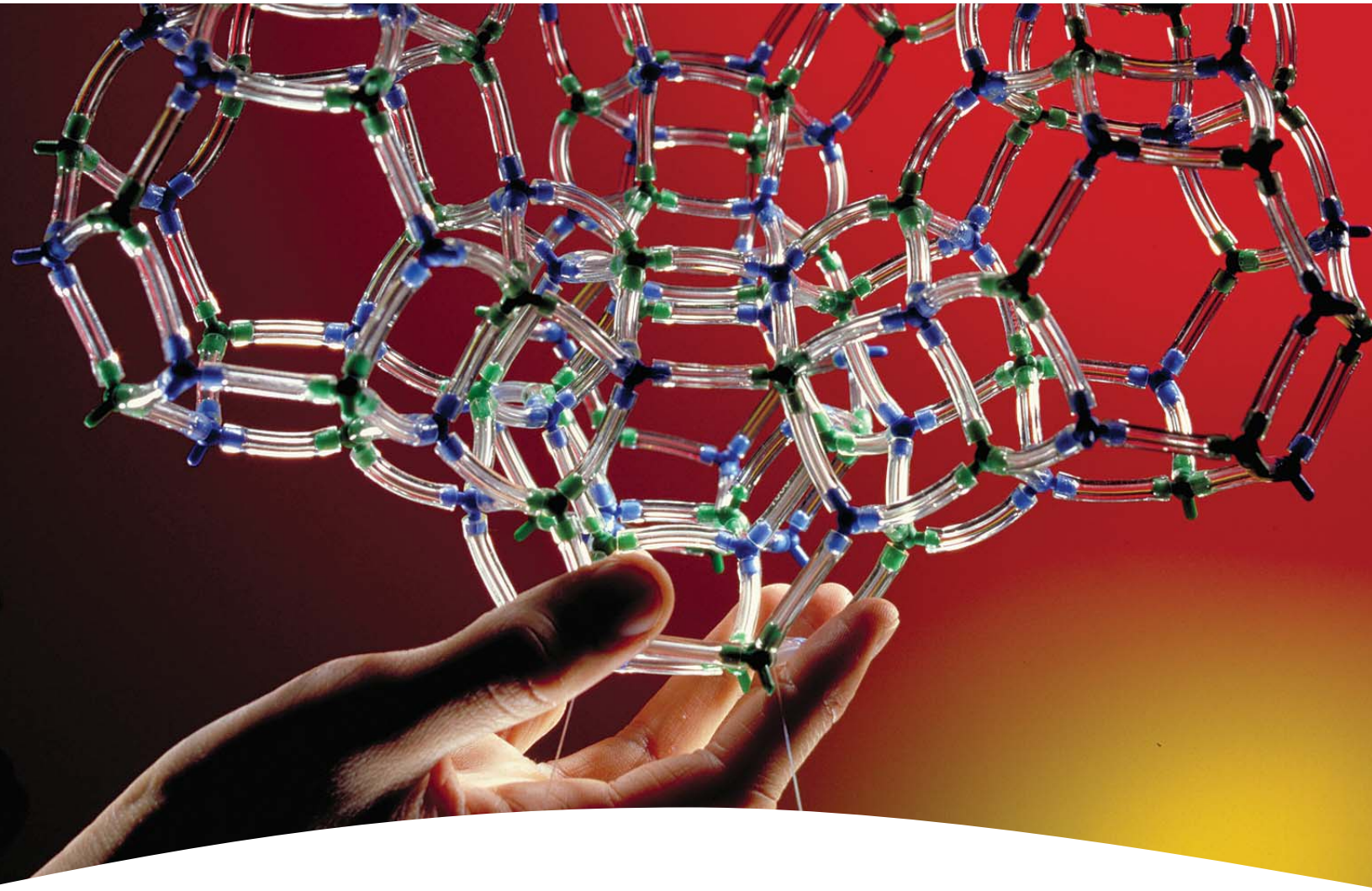
UOP Adsorbents



UOP molecular sieves in urethane systems

A Honeywell Company

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Applications

The unusual physical properties of polyurethane resins have resulted in their wide acceptance in applications where outstanding performance is required. Their fine gloss retention, wear resistance, weathering, and adhesive properties make them preferred resins for protective coatings, floor coverings, sealants, and caulks. For several applications, however, their rapid reactivity with water requires that precautions be taken to provide for the development of these properties. Premature reaction with water can cause gassing during storage or viscosity buildup in storage containers. This can be prevented by incorporating UOP molecular sieves in urethane formulations. They reduce gassing during storage, insure flowable reactants, and give a denser more durable cured polymer.

In many plastic and polymer systems our molecular sieves perform a dual role to a great advantage. First, they scavenge trace moisture from the formulation to give a longer shelf life with no pressure development. Second, they have the capacity to adsorb water present during application. Such water is always present on the surface of concrete, steel, tile, etc. to which the urethane formulation is being applied, and can be trapped beneath the urethane coating. There it reacts with the isocyanate group (NCO) to form CO_2 gas which greatly decreases urethane hardness. UOP molecular sieves can prevent this thereby making it possible to formulate a stable one package system which cures with superior properties.

UOP molecular sieves are synthetic crystalline metal aluminosilicates which have within their crystal structure a very high surface area and a uniform pore system. Water is adsorbed preferentially over all other compounds, illustrated by their strong advantage in “scavenging” water in polyurethane systems. The water, once adsorbed within the crystalline pore system, is retained there and isolated from the resin formulation, thereby providing resin dryness. UOP molecular sieve powder is essentially inert to the other formulation components. Our molecular sieve powders have already been successfully employed to prevent gassing, gelation, erratic viscosity, and other problems in adhesive, sealant, coating, plastic, and rubber systems.

Physical and Chemical Properties	
UOP MOLSIV™ 5A adsorbent	$Ca_{4.5}\ Na_3\ (AlO_2)_{12}(SiO_2)_{12}$
Appearance	White powder
Bulk density	30 lb/ft^3
Particle size	1-5 Microns
Heat of adsorption	1800 Btu/lb H_2O (Max.)
Storage stability of powder	Good if normal precautions are taken to exclude moisture
Toxicity	Avoid breathing dust and prolonged or repeated skin contact. In case of contact with eyes, immediately flush with water for at least 15 minutes.

Coatings

One component moisture cured polyurethane systems have long been used because of their low toxicity and ease of use. However, the incorporation of pigments and solvents causes many problems because of trace moisture quantities present. UOP molecular sieves, by removing trace quantities of moisture introduced with pigments and solvents, make it easy to formulate one or two component, pigmented or non-pigmented, polyurethane coatings.

Stable, non-gassing polyurethane coatings can be prepared as shown in formulation A and C of **Table 1** (next page).

In preparing formulations A and C, the pigment, dried solvent, and UOP 5A adsorbent powder were ball mill ground for two hours. The castor oil prepolymer was then added and grinding was continued until the desired fineness of grind was obtained. No pressure build up occurred in the ball mill and a low viscosity product was obtained. The formulations without molecular sieve powder (formulation B and D) built up considerable pressure in the ball mill and gave a high viscosity product. UOP molecular sieves protected against gassing in both the castor oil and the oil-free system.

The quantity of molecular sieve powder incorporated into the pigment and solvent slurry is based on the measured water content of the ingredients. The amount recommended is about 5-15 times the water content. Because the vapor pressure of water over molecular sieves is a function of the water loading, enough molecular sieve powder is added to reduce the vapor pressure below the threshold value. For best results, UOP molecular sieve powder and pigment should be mixed prior to adding the prepolymer.

Table 1

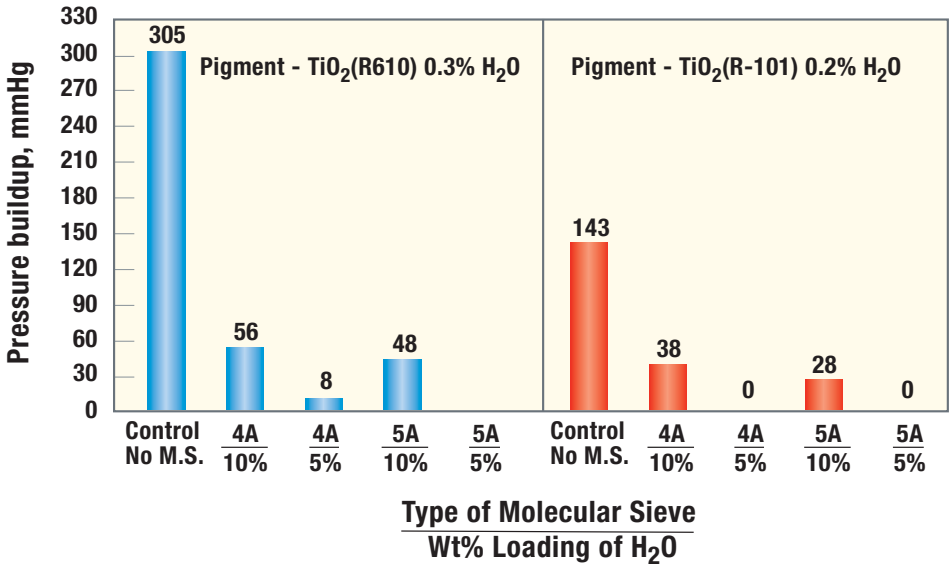
Effect of UOP MOLSIV 5A Adsorbent Powder on Polyurethane Coating Formulations

Ingredients, gms	A	B	C	D
TiO_2[a]	146	146	146	146
Xylene[b]	172.5	172.5	—	—
P-93-100[c]	181.5	181.5	—	—
DV-1180[d]	—	—	363	363
UOP 5A adsorbent	2.9	—	2.9	—
Results				
Viscosity (Poises)				
Initial	4.0	22.0	2.6	2.6
9 Months	12.0[e]	40.0[e]	12.0[e]	24.0[e]
Ball mill gassing	None	Considerable	None	Considerable

a. Grade R-101 (0.2% H_2O), E.I. duPont de Nemours and Company Inc.
b. Predried with UOP MOLSIV™ 4A beads.
c. Polyurethane castor oil prepolymer (8% NCO), Spencer Kellogg and Sons, Inc.
d. Polyurethane prepolymer, no oil, 50% NV (4.7% NCO), Spencer and Kellogg and Sons, Inc.
e. Can was opened to air several times, thus accounting for some increase in viscosity
f. Partial gelation noted in 2 months.

Figure 1

Effect of Molecular Sieve Powder on Gas Evolution of Polyurethane Sealant Formulations



Urethane Sealants

Polyurethane compounds used as sealants (caulks) generally contain little or no solvents but have a high content of fillers and pigments. Preparation and storage of these compounds has been extremely difficult because of excessive gassing and gelation of the product. Almost all pigments and fillers contain some degree of residual moisture which, when mixed with urethanes, causes gassing and gelation. UOP molecular sieves effectively and easily remove all trace amounts of moisture from fillers, pigments, and polyol thus preventing gassing, foaming, and pre-gelling.

Predrying the pigment with molecular sieve powder prior to prepolymer addition gives stable non-gassing formulations. The effect of molecular sieve concentration on gas evaluation in a urethane sealant system is shown in **Figure 1**. The control formulation containing no molecular sieve developed a pressure of over 300 mm Hg. The samples containing molecular sieve with total water adsorption loading of 5% and 10% developed little or no pressure build up.

The formulation in **Table 2** was tested for gassing and gelation at 120°F using calcium sulfate, silica gel and our UOP molecular sieves as desiccants.

Table 2

Urethane Sealant Formulation Used to Test Various Desiccants

Ingredients	
XP-1418[a]	100.00
TiO_2	15.4
Calcium Carbonate	67.5
Toluene	2.2

a. Polyurethane prepolymer (3.1% NCO), Spencer Kellogg Division of Textron, Inc.

The same formulation was used in each test and storage was in a sealed container at 120°F. With 0.1% water initially present in each formulation, the pressure buildup in each container during storage is shown in **Figure 2**. All systems using other desiccants (3% silica gel or 10% calcium sulfate) gelled in a short period of time. The silica gel system also exhibited extreme gassing. Pressure buildup ceased when gelation occurred since the gas could no longer escape from the dense cross-linked urethane. The example with one weight percent UOP 5A molecular sieve powder neither gassed nor gelled — the protection offered by the molecular sieves was complete.

Figure 2
Gassing In A Gun-Grade Urethane Sealant Formulated with Various Desiccants

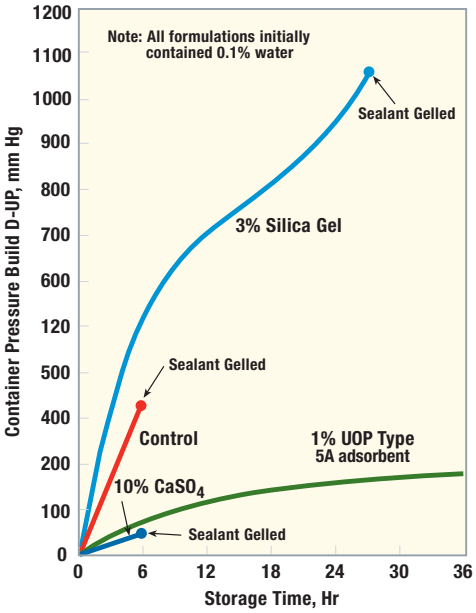


Table 3
Typical Polyester-Castor Oil Urethane Floor Formulation

Part	Component	Weight	Description
A-Polyol	"Multron" R-12	50	Mobay-Polyester polyol
	Castor Oil	50	Anhydrous grade
	$CaCO_3$	106	Filler
	Molecular sieve	2	UOP MOLSIV 3A adsorbent powder
	Pigment	As desired	Anhydrous
B-Isocyanate	"Mondur" MR	42	Mobay-Polyisocyanate

Urethane Flooring

Urethane flooring can be formulated to produce a seamless, continuous surface with the outstanding properties of the urethane polymers. This solvent-free system has the distinct advantages of having no solvent loss, and making possible the renovation of existing tile floors without removing the old tile.

The general purpose formulation shown in **Table 3** was developed based on a polyester resin isocyanate prepolymer and castor oil. The system can be successfully applied over a wide range of humidity conditions. It exhibits a favorable combination of flexibility and hardness. Where greater abrasion and scratch resistance is required, a clear urethane top coat provides good results.

The molecular sieve in the system insures a free, flexible formulation with excellent flooring properties. Without UOP molecular sieve, the residual moisture, which is always present on surfaces to be coated, reacts readily with the isocyanate groups of the resin to produce carbon dioxide. If enough moisture is present bubbles appear which reduce abrasion resistance. Even if trace amounts of moisture are present, and the resultant carbon dioxide is insufficient to from bubbles, the presence of these small quantities of carbon dioxide will reduce abrasion resistance and hardness of the finished floor. UOP molecular sieves prevent the formation of carbon dioxide thus making possible floors which have both better abrasion resistance and increased hardness.

Find out more

If you are interested in learning more about our UOP adsorbents please contact your UOP representative or visit us online at www.uop.com

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