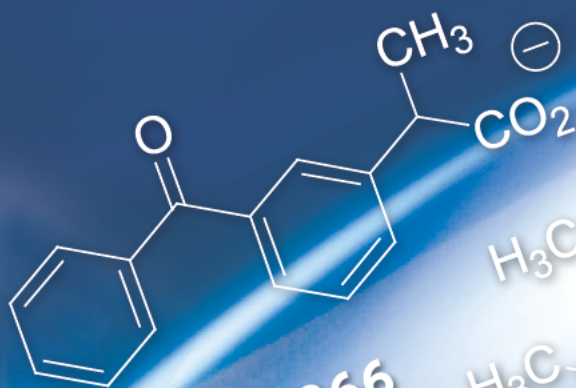
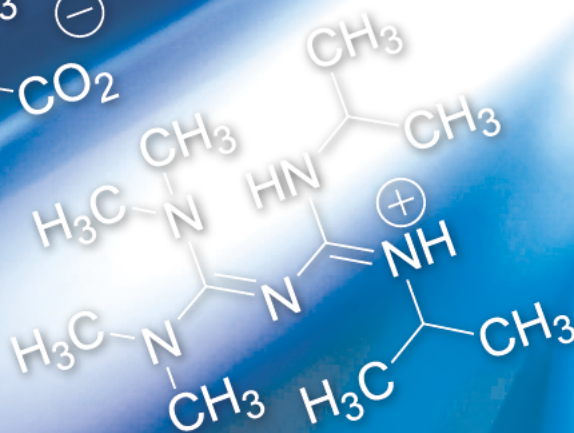


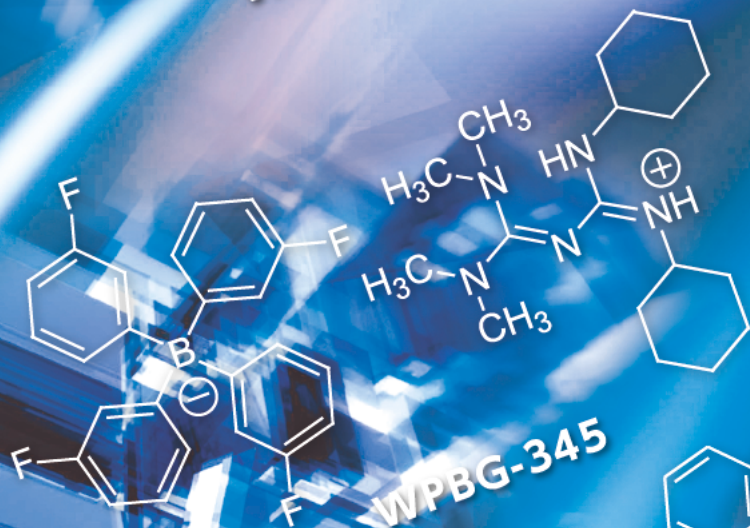
Photo Base Generators



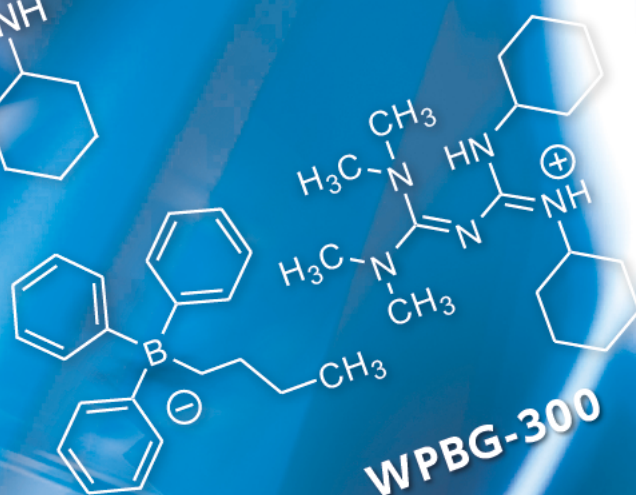
WPBG-266



WPBG-300



WPBG-345



Index	Introduction..... P1	WPBG-300 P9-12	WPBG-165 P18
	Different Reactions using Bases ... P2	WPBG-345 P13-15	WPBG-027 P19
	Selection Guide..... P3,4	WPBG-018 P16	PBG Reagent List P20
	WPBG-266 P5-8	WPBG-140 P17	List of related Items P21-22

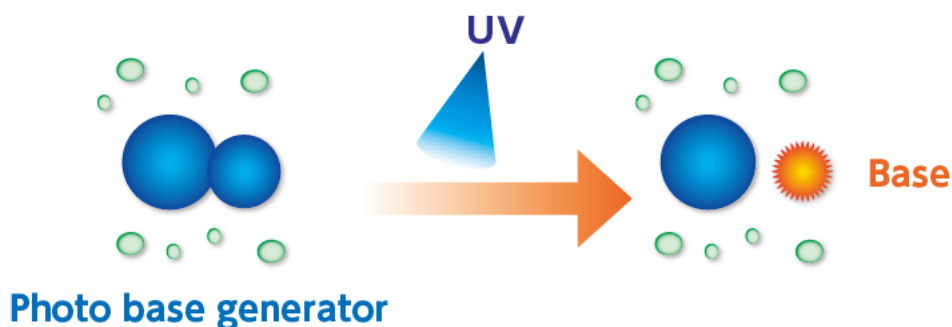
Introduction

We have developed different types of polymerization initiators by establishing novel organic synthetic technologies, manufacturing techniques and refining technologies accumulated through our extensive experience in reagent manufacturing. The photo base generators are used as reaction initiators in the synthesis of polymers. The technology can be applied in different areas including coating materials and sealants for electronics equipment.

What is a Photo Base Generator, or PBG?

A Photo base generator is a compound which generates organic base such as amines upon irradiation of light in the UV range.

The generated organic base accelerates an anionic UV curing of epoxy resin, sol-gel method, etc.



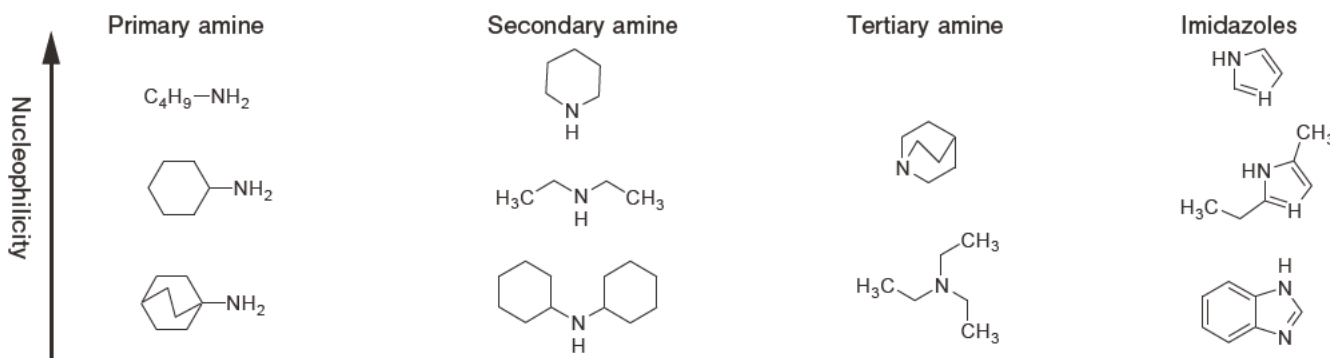
Characteristics of anionic polymerization

- (i) Can be used in air.
(No disturbance of curing)
- (ii) Can conduct delay cure.
(Anion of active species is not deactivated)
- (iii) Can be used on metal wiring.
(Hardly causes metallic corrosion)

Active Species	Example of Reaction	Inhibition	Delay cure	Metallic Corrosion
Radical		O ₂	Non	Non
Cationic		H ₂ O	Yes	Yes
Anionic		Non	Yes	Non

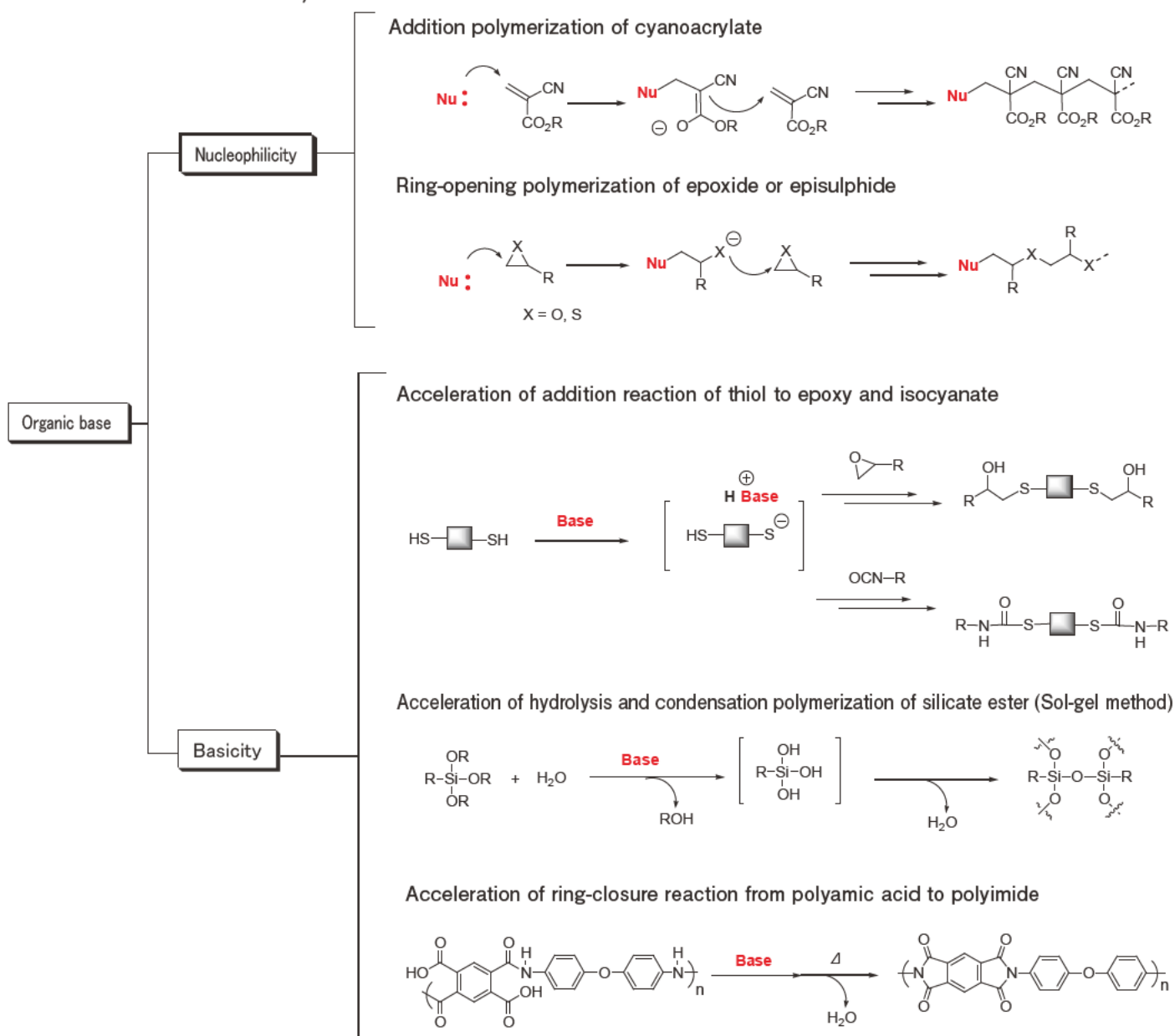
Typical organic base

Organic bases which are generated by UV irradiation have "nucleophilicity" and "basicity". These bases function as initiators to promote different reactions.

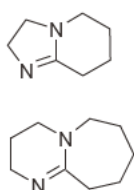


Different reactions utilizing bases

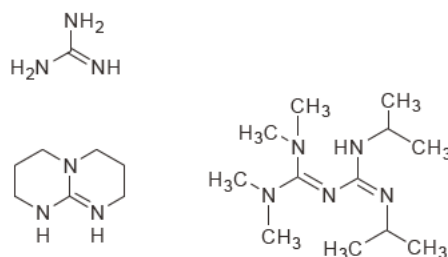
Organic bases are able to initiate different curing reactions by utilizing their nucleophilicity and basicity. Bases are also available for purposes other than curing agents. For example, as a catalyst for depolymerization and neutralizer for acidic systems.



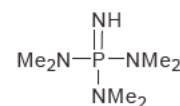
Amidines



Guanidines



Phosphazenes



Basicity →

*We do not necessarily line up all the bases described here.

*This chart shows only images, which do not express their accurate physical properties.

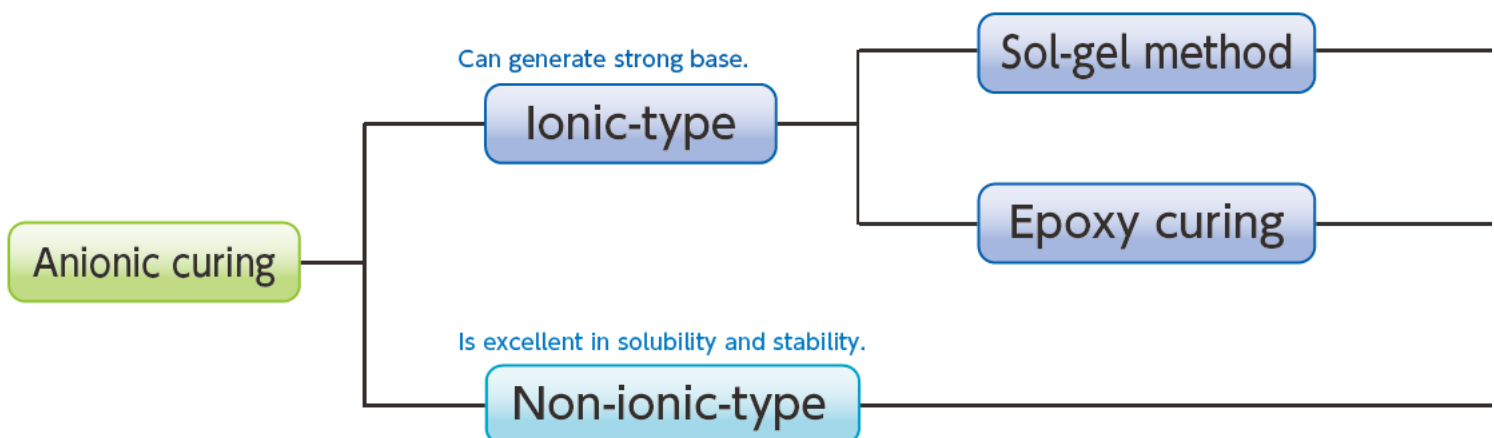
Selection guide

PBG materials are largely classified into “Ionic type” and “Non-ionic type” by their structure.

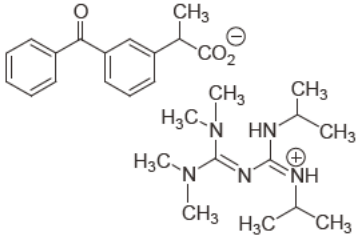
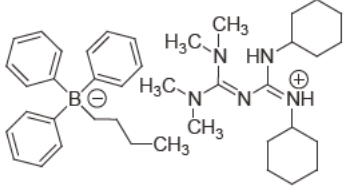
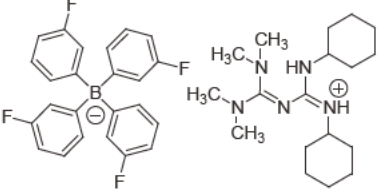
- Ionic-type PBG generates strong organic bases such as tertiary amines, amidines and guanidines. Ionic-type PBG materials are characterized by high reactivity with cross-linking agents and monomers.
- Non-ionic type PBG materials generate primary and secondary amines and imidazoles, and are characterized by excellent stability and heat resistivity.

Step 1 Ionic-type or Non-ionic-type?

Step 2 For what application?

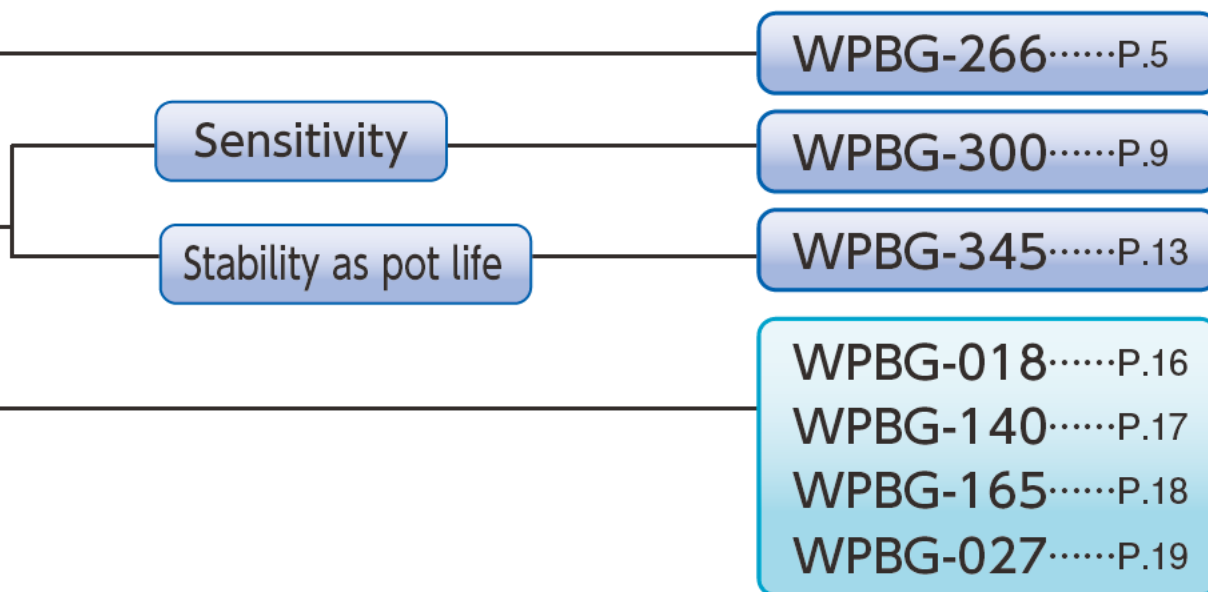


Ionic-type PBG

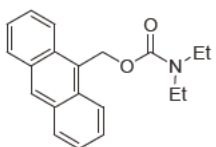
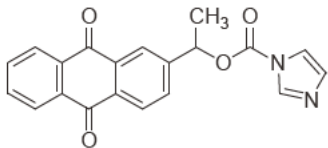
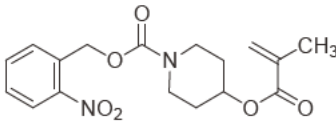
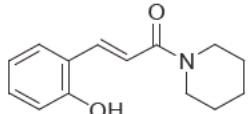
	Products	Strong Base	Solubility	Stability	irradiation @365 nm	Sensitizer	Page
Carboxylate	 <p>WPBG-266</p>	Yes	Yes	Non	Non	Non	P.5-8
Borate	 <p>WPBG-300</p>	Yes	Yes	Yes	Non	Yes	P.9-12
	 <p>WPBG-345</p>	Yes	Yes	Yes	Non	Yes	P.13-15

Select the most suitable products based on the type of generated base, solubility for resin (and solvent/diluent), stability as pot life, UV absorption wavelength, etc.

Step 3 What do you value?



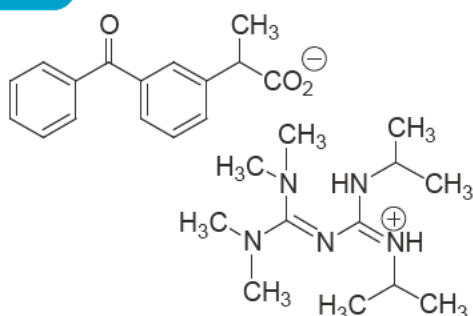
Non-ionic-type PBG

	Products	Strong Base	Solubility	Stability	irradiation @365 nm	Sensitizer	Page
Carbamate	 WPBG-018	Non	Yes	Yes	Yes	Non	P.16
	 WPBG-140	Non	Non	Non	Yes	Non	P.17
	 WPBG-165	Non	Yes	Non	Non	Yes	P.18
Amide	 WPBG-027	Non	Non	Yes	Yes	Non	P.19

WPBG-266

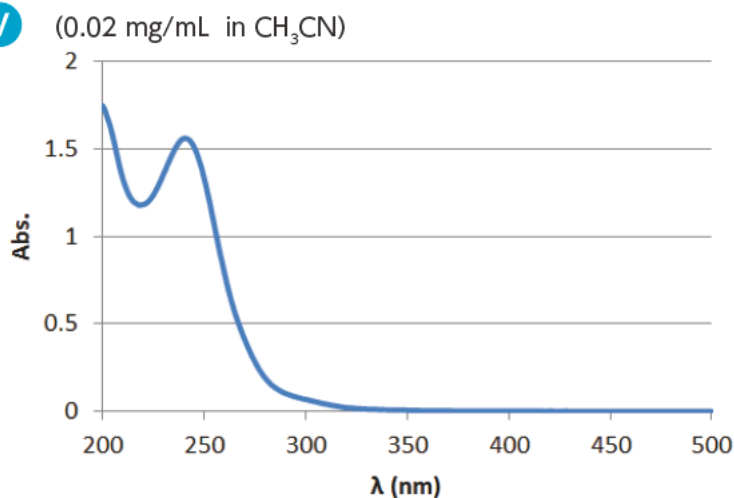
Chemical name | 1,2-Diisopropyl-3-[bis(dimethylamino)methylene]guanidium 2-(3-benzoylphenyl)propionate

Structural



Formula	$C_{28}H_{41}N_5O_3$
Molecular weight	495.66
CAS No.	1632211-89-2
Melting point	115°C
TG-DTA	weight loss from 191°C
Appearance	white powder
TSCA	Not Listed
EINECS	Not Listed

UV



Absorption maximum

240 nm ($\epsilon=34000$)

254 nm ($\epsilon=25400$)

365 nm ($\epsilon=80$)

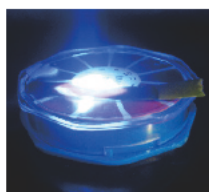
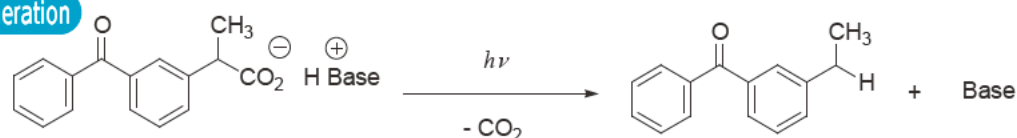
Solubility (g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
25	18	7	24	42	44	73	45
Si(OEt) ₄		Me-Si(OMe) ₃		Ph-Si(OMe) ₃		HS-C ₃ H ₆ -Si(OMe) ₃	
3		3		6		8	

Characteristics

- Generates a strong base, biguanide ($pK_{bH}=31.8$), in high quantum yield upon irradiation.
- Shows high solubility to various solvents.
- Has radical initiation capability.
- Is optimal as catalyst for sol-gel method.

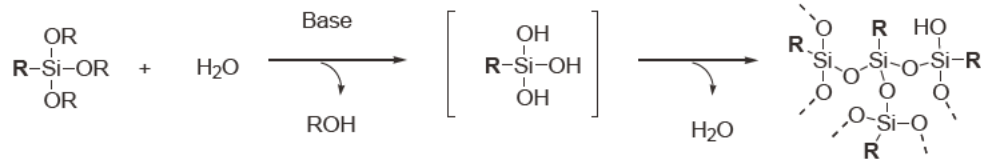
Mechanism of base generation



Immerse pH-test paper in the aqueous solution, irradiate UV, and the transition to the basicity is confirmed visually.

Sol-gel method

The Sol-gel method is a technique to form metal oxides by hydrolysis and condensation polymerization of alkoxysilane, etc. It is generally well known that both hydrolysis and condensation polymerization proceed promptly when bases are used.



WPBG-266 is optimal for the curing of the silanol compounds formed by hydrolysis of trisubstituted alkoxysilyl compounds. The silanol compounds formed by hydrolysis of tetrasubstituted alkoxysilyl compounds tend to gel easily, therefore they must be handled carefully.

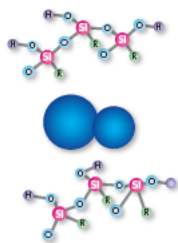
Example of Use 1

Anionic UV curing of methyl/phenyl silicone resin

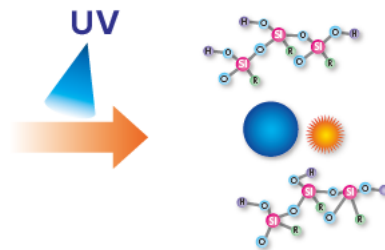
KR-300 is a high-temperature-curing-type silanol polymer having methyl and phenyl groups on a silicon atom. Curing temperature can be decreased by using WPBG-266 combined with light exposure.

Before curing

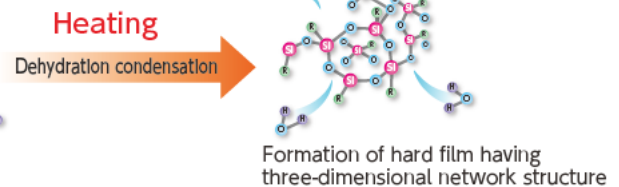
WPBG + silicone resin



Generation of strong base



After curing



Conditions

Composition: 5 parts of WPBG-266, 100 parts of 2-isopropylalcohol and 100 parts of KR-300 (Product of Shin-Etsu Chemical Co., Ltd.) are blended.

Film-forming: Glass plate (i) Spin coat: 500 rpm/5 seconds → 1000 rpm/30 seconds

(ii) Pre-bake: 80°C/1 minute

Film thickness: approximately 10 μm

Exposure: Irradiate for 10 seconds (Illuminance: 5 mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Post-exposure bake: 150°C/5 minutes

Results

Solvent resistance of cured film: Acetone, MEK, ethanol, and IPA

Thermogravimetric measurement (200°C): The cured material obtained by the above process: -0.26%

Reference example The cured material obtained by the process of 250°C/60 minutes: -0.34%

Equivalent cured material can be obtained under low temperature and in a short time of period.

Effect of post-exposure baking (PEB):

PEB(°C)	0min	5min	10min	20min	30min	40min	60min	90min
80								
100								
120								
150								

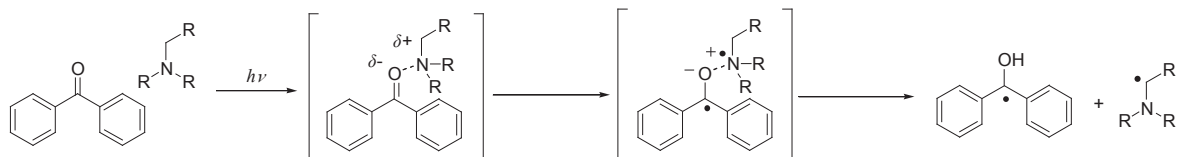
Development by acetone is possible. High contrast is obtained.

Completely cures and is insoluble in solutions of acetone, MEK, etc.

*The above composition is only a reference example, We do not guarantee the physical properties.

■ Mechanism of radical generation from WPBG-266.

WPBG-266 is able to generate two different active species a base and a radical by light irradiation. radical with light irradiation.

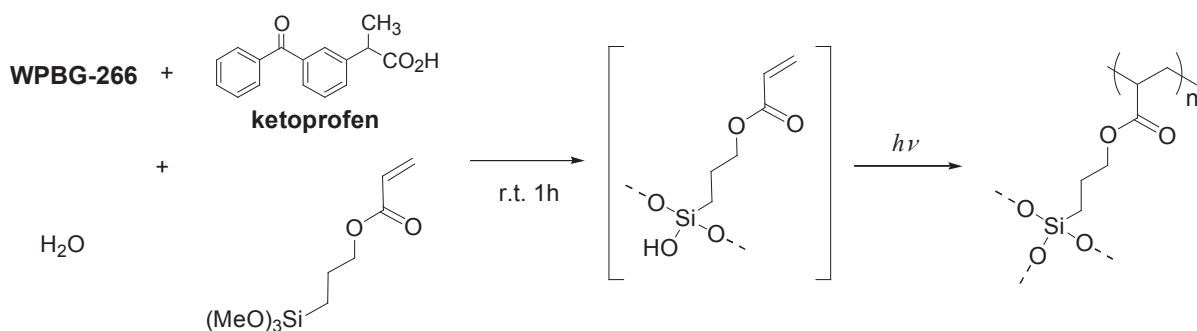


■ Hydrolysis using WPBG-266 with ketoprofen (a carboxylic acid which decarboxylates by light irradiation)

The hydrolysis of silane coupling agents in the presence of WPBG-266, ketoprofen and water will be accelerated by the lower pH (acidic conditions). The silanol body thus obtained is not isolated and the system moves to basicity if UV is irradiated as it is. Therefore, cured material can be formed from one component.

Example of Use 2

■ UV curing using radical polymerization and sol-gel method together (organic and inorganic hybrid)



Conditions

Preparation: Mix 15 parts of WPBG-266, 5 parts of ketoprofen, 245 parts of (3-acryloxy)propyltrimethoxysilane, and 54 parts of water and stir the solution until it becomes homogeneous at the room temperature.

Film-forming: After application with a wire bar, prebake at 80°C/1 minute.

Film thickness: approximately 10-20 μm

Exposure: Under N_2 flow, irradiate for 30 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Post-exposure bake: None

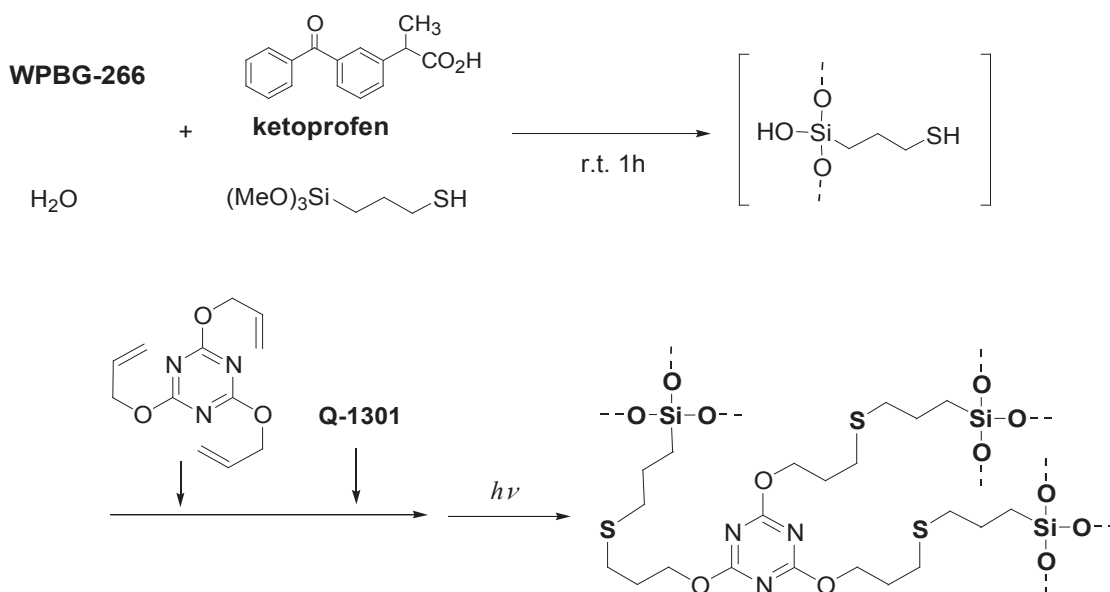
Results

Pencil hardness test : 6H or more

Abrasion-resistant test : No scratch with steel wool #0000

Example of Use 3

■ UV curing using thiol-ene reaction together with the sol-gel method (organic and inorganic hybrid)



Conditions

Preparation: Mix 15 parts of WPBG-266, 5 parts of ketoprofen, 196 parts of (3-mercaptopropyl)trimethoxysilane, and 27 parts of water and stir the solution until it becomes homogeneous at the room temperature. Add 83 parts of 2,4,6-tris(allyloxy)-1,3,5-triazine and 0.3 part of polymerization inhibitor Q-1301 (Product of FUJIFILM Wako Pure Chemical Corporation) and mix.

Film-forming: After application with a wire bar, prebake at 80°C/1 minute.

Film thickness: approximately 10-20 μm

Exposure: Irradiate for 10 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Post-exposure baking: None

Results

Pencil hardness test: Glass: 6H or more, Polycarbonate: H

Abrasion-resistant test: No scratch with steel wool #0000

Reference

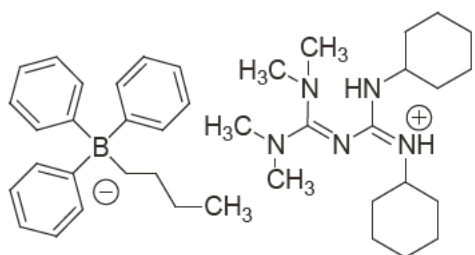
- K. Arimitsu, A. Kushima, *et al.*, *Polymer Preprints, Japan*, **2005**, *54*, 1357.
- K. Arimitsu, A. Kushima, R. Endo, *J. Photopolym. Sci. Technol.*, **2009**, *22*, 663.
- K. Arimitsu, R. Endo, *Chem. Mater.* **2013**, *25*, 4461-4463.
- K. Arimitsu, *Journal of Synthetic Organic Chemistry, Japan* **2012**, *70*, 508.

*The above composition is only a reference example, We do not guarantee the physical properties.

WPBG-300

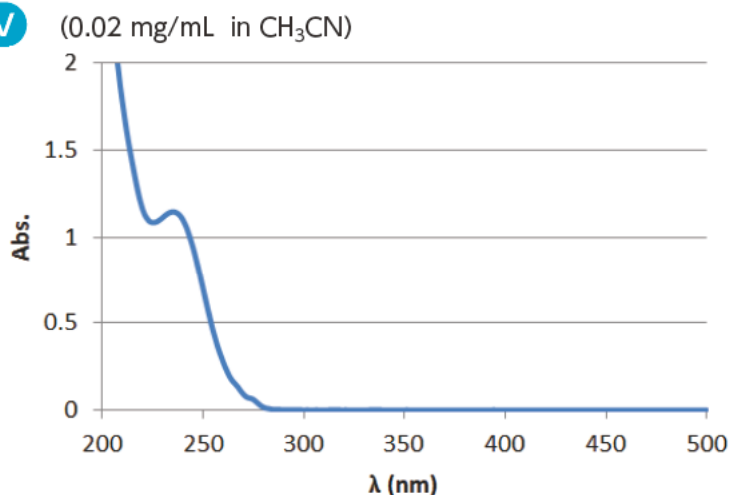
Chemical name | 1,2-Dicyclohexyl-4,4,5,5-tetramethylbiguanidium *n*-butyltriphenylborate

Structural



Formula	C ₄₀ H ₆₀ BN ₅
Molecular weight	621.75
CAS No.	1801263-71-7
Melting point	115°C
TG-DTA	weight loss from 203°C
Appearance	white powder
TSCA	Not Listed
EINECS	Not Listed

UV



Absorption maximum

197 nm ($\epsilon=79000$)254 nm ($\epsilon=14000$)365 nm ($\epsilon=0$)

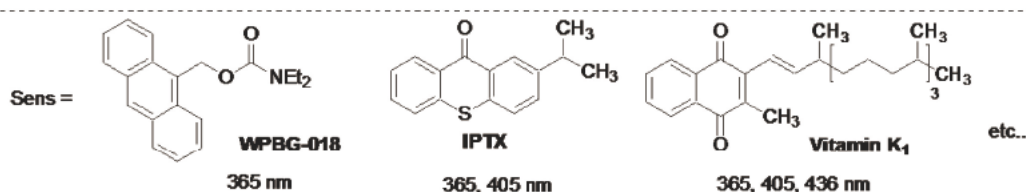
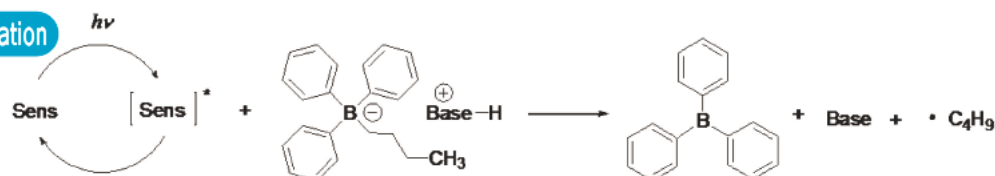
Solubility (g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
29	41	5	46	8	7	4	<0.5

Characteristics

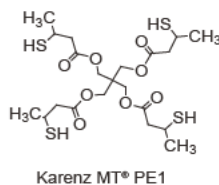
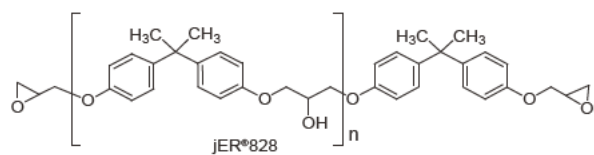
- Shows high stability (pot life) in monomer.
- Generates a strong base, biguanide (pK_{bH}=31.8), upon irradiation.
- Can be exposed with sensitizer at 365 nm and longer wavelength.
- Can be employed with cross-linking agents such as thiol or anhydride.

Mechanism of base generation



Example of Use 1

■ Anionic UV curing of epoxy oligomer × polyfunctional thiol



Conditions

Preparation: Mix 1-5 parts of WPBG 300, 0.2-1 part of 2-isopropylthioxanthone (0.2 equivalent amount to WPBG), and 100 parts of jER®828 (epoxy equivalent of 185, Product of Mitsubishi Chemical Corporation), and heat or use a diluent to promote dissolution. Mix 70 parts of KarenzMT®PE1 (SH equivalent of 138.5, Product of Showa Denko K.K.) at room temperature.

Stability of composition as pot life (period in which the viscosity does not exceed the twice of the initial viscosity): 1 month (10°C), 1 week (25°C), and 3 days (40°C)

Exposure: Irradiation for 10 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Results

Post-exposure bake:

	PEB(°C)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 1 part	50									
	80									
	100									
	120									
	150									
PBG 3 parts	50									
	80									
	100									
	120									
	150									
PBG 5 parts	50									
	80									
	100									
	120									
	150									

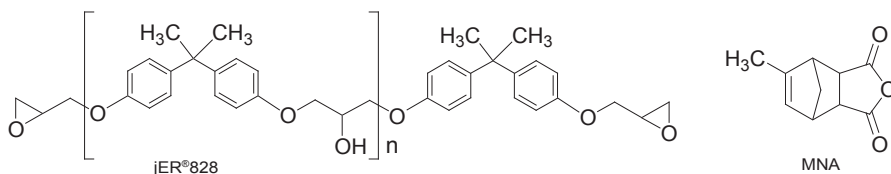
Effect of exposure amounts: Post-exposure bake at a fixed temperature of 80°C

	PEB(°C)	80°C									
		Exposure value (J/cm ²)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 1 part	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										
PBG 3 parts	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										
PBG 5 parts	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										

Color	Exposure	Unexposure
	Liquid	Liquid
	Thick	Liquid
	Cured	Liquid
	Cured	Cured

Example of Use 2

■ Anionic UV curing of epoxy oligomer × acid anhydride



Conditions

Preparation: Mix 3-10 parts of WPBG-300, 0.6-2 parts of 2-isopropylthioxanthone (0.2 equivalent amount to WPBG), and 100 parts of jER®828 (epoxy equivalent of 185, Product of Mitsubishi Chemical Corporation), and heat or use a diluent to dissolve.

Mix 50 parts of methyl-5-norbornene-2,3-dicarboxylic anhydride (Product of FUJIFILM Wako Pure Chemical Corporation) at room temperature.

Stability of composition as pot life (period in which the viscosity does not exceed the twice of the initial viscosity): 1 month or more (10°C), 2 weeks (25°C), and 3 days (40°C)

Exposure: Irradiation for 10 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Results

Post-exposure bake:

	PEB (°C)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 3 parts	100									
	120									
	150									
	170									
PBG 5 parts	100									
	120									
	150									
	170									
PBG10 parts	100									
	120									
	150									
	170									

Effects of exposure amounts: Post-exposure bake at a fixed temperature of 150°C

PEB (°C) \ Exposure value (J/cm ²)	150°C									
	0min	5min	10min	20min	30min	40min	60min	90min	120min	
PBG 3 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									

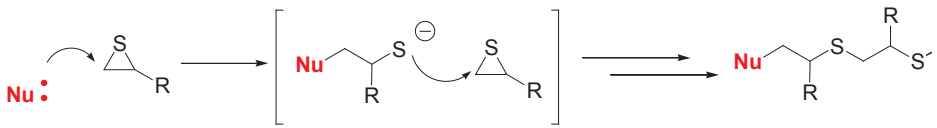
PEB (°C) \ Exposure value (J/cm ²)	150°C									
	0min	5min	10min	20min	30min	40min	60min	90min	120min	
PBG 5 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									

PEB (°C) \ Exposure value (J/cm ²)	150°C									
	0min	5min	10min	20min	30min	40min	60min	90min	120min	
PBG10 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									

Color	Exposure	Unexposure
	Liquid	Liquid
	Thick	Liquid
	Cured	Liquid
	Cured	Cured

Example of Use 3

■ Anionic UV curing of episulfide



Conditions

Preparation: Mix 1-5 parts of WPBG-300 and 0.2-1 part of 2-isopropylthioxanthone (0.2 equivalent amount to WPBG) in 20 parts of γ -butyrolactone and mix hydrogenated bisphenol A type episulphide (episulphide equivalent of 220).

Stability of components as pot life (period in which the viscosity does not exceed the twice of the initial viscosity): 3 weeks (10°C), 2 weeks (25°C), and 3 days (40°C)

Exposure: Irradiation for 10 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Results

Post-exposure bake:

	PEB(°C)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 1 part	50									
	80									
	100									
	120									
	150									
PBG 3 part	50									
	80									
	100									
	120									
	150									
PBG 5 part	50									
	80									
	100									
	120									
	150									

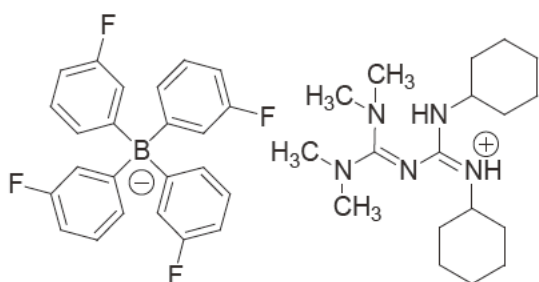
Effect of exposure amounts: Post-exposure bake at a fixed temperature of 80°C

	PEB(°C)	80°C									
		Exposure value (J/cm ²)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 1 part	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										
PBG 3 part	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										
PBG 5 part	0.1										
	0.3										
	0.5										
	1										
	2										
	5										
	10										

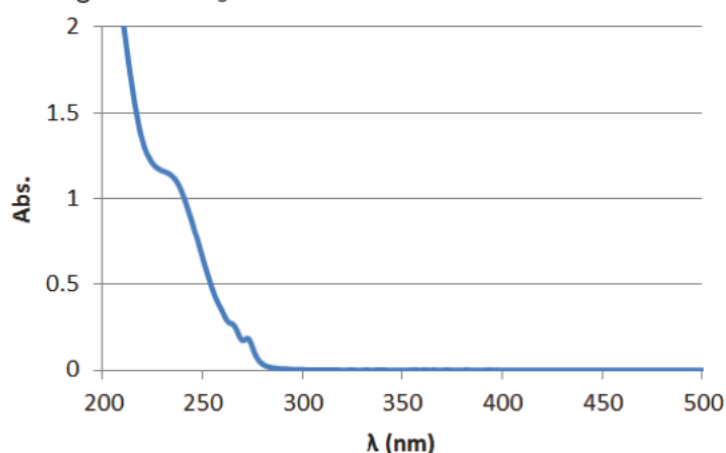
Color	Exposure	Unexposure
	Liquid	Liquid
	Thick	Liquid
	Cured	Liquid
	Cured	Cured

WPBG-345

Chemical name (Z)-[[Bis(dimethylamino)methylidene]amino]-N-cyclohexyl(cyclohexylamino)methaniminiumtetrakis(3-fluorophenyl)borate

Structural

Formula	C ₄₂ H ₅₂ BF ₄ N ₅
Molecular weight	713.70
CAS No.	2073916-67-1
Melting point	138°C
TG-DTA	weight loss from 231°C
Appearance	nearly white crystals
TSCA	Not Listed
EINECS	Not Listed

UV(0.02 mg/mL in CH₃CN)

Absorption maximum

197 nm ($\epsilon=118000$)254 nm ($\epsilon=15500$)365 nm ($\epsilon=15$)**Solubility**

(g/solv. 100 g)

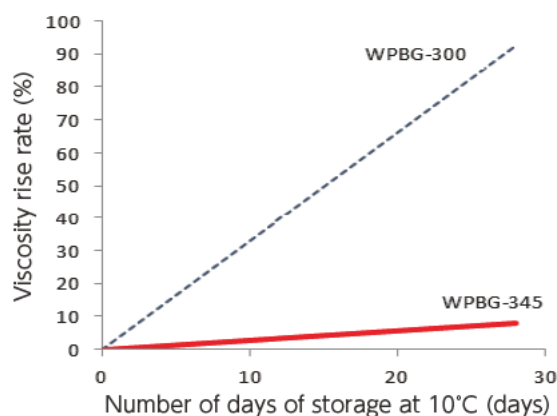
NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
62	81	55	107	31	44	3	<0.5

Characteristics

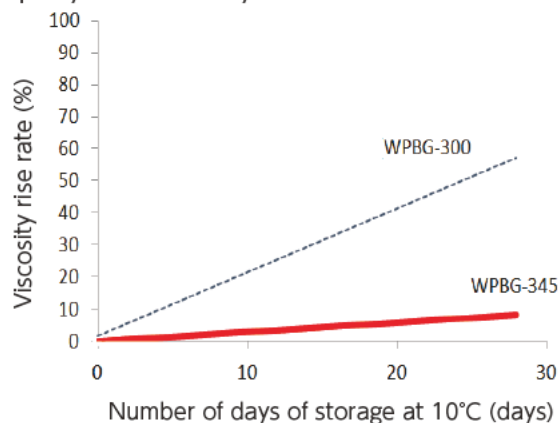
- Shows high stability (pot life) in various compositions (epoxy × thiol and epoxy × acid anhydride).
- Generates a strong base, biguanide ($pK_{bH}=31.8$), upon irradiation.
- Can be exposed with sensitizer at 365 nm and longer wavelength.

Stability of compositions as pot life

Epoxy × thiol



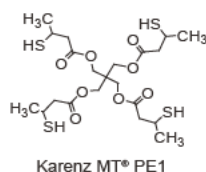
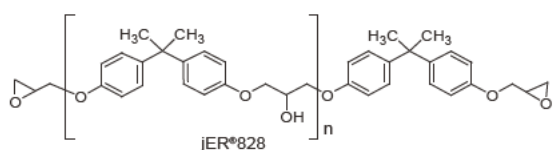
Epoxy × Acid anhydride



- Possible to use sensitizer in order to irradiate @365 nm and longer wavelength.
- higher stability of pot-life than WPBG-300.

Example of Use 1

■ Anionic UV curing of epoxy oligomer × polyfunctional thiol



Conditions

Preparation: Mix 3-10 parts of WPBG-345, 0.6-2 parts of 2-isopropylthioxanthone (0.2 equivalent amount to WPBG), and 100 parts of jER®828 (epoxy equivalent of 185, Product of Mitsubishi Chemical Corporation), and heat or use a diluent to promote dissolution. Mix 70 parts of KarenzMT®PE1 (SH equivalent of 138.5, Product of Showa Denko K.K.) at room temperature.

Stability of components as pot life (period in which the viscosity does not exceed the twice of the initial viscosity): 2 month or more (10°C), 3 weeks (25°C), and 3 days (40°C)

Exposure: Irradiation for 10 seconds (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Results

Post-exposure bake: Illuminance 1.0 J/cm² (@365 nm)

	PEB (°C)	0min	5min	10min	20min	30min	40min	60min	90min	120min
PBG 3 parts	50									
	80									
	100									
	120									
	150									
PBG 5 parts	50									
	80									
	100									
	120									
	150									
PBG 10 parts	50									
	80									
	100									
	120									
	150									

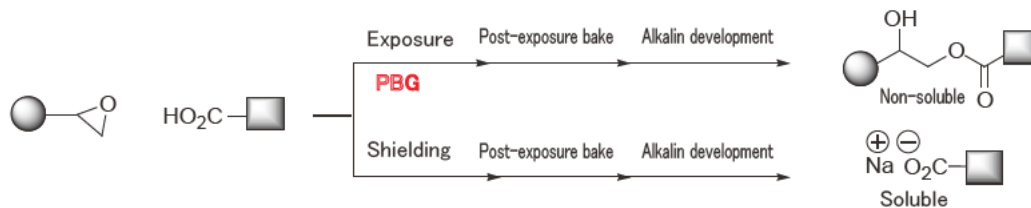
Effect of exposure amounts: Post-exposure bake at a fixed temperature of 120°C

	PEB (°C)	120°C								
		Exposure value (J/cm ²)	0min	5min	10min	20min	30min	40min	60min	90min
PBG 3 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									
PBG 5 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									
PBG 10 parts	0.1									
	0.3									
	0.5									
	1									
	2									
	5									
	10									

Color	Exposure	Unexposure
	Liquid	Liquid
	Thick	Liquid
	Cured	Liquid
	Cured	Cured

Example of Use 2

■ Patterning by epoxy oligomer × carboxylic acid



Conditions

Preparations: Mix 1-10 parts of WPBG-345, 0.2-2 parts of 2-isopropylthioxanthone (0.2 equivalent amount to WPBG), and 100 parts of jER®828 (epoxy equivalent of 185, Product of Mitsubishi Chemical Corporation) and 64 parts of Joncryl®682 (OH equivalent of 138, Product of BASF Japan Ltd.) into 300 parts of γ -butyrolactone.

Film-forming: Polycarbonate, film thickness: 10-20 μ m

Exposure: Optional (Illuminance: 5mW/cm² (254 nm), 100 mW/cm² (365 nm), and 261 mW/cm² (405 nm))

Post-exposure bake: 150°C/10 minutes

Development: 1 wt% Na₂CO₃, Immerse for 1 minute → rinse with water.

Results

Effects of exposure amounts:

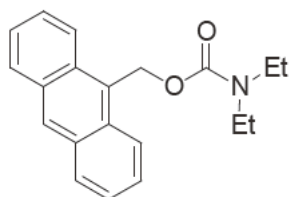
PBG 1 part	Exposure value (J/cm ²)	0.1	0.3	0.5	1	2	5	10
	Existence of remaining film							
PBG 3 parts	Exposure value (J/cm ²)	0.1	0.3	0.5	1	2	5	10
	Existence of remaining film							
PBG 5 parts	Exposure value (J/cm ²)	0.1	0.3	0.5	1	2	5	10
	Existence of remaining film							
PBG 10 parts	Exposure value (J/cm ²)	0.1	0.3	0.5	1	2	5	10
	Existence of remaining film							

Color	Exposure	Unexposure
	Liquid	Liquid
	Thick	Liquid
	Cured	Liquid

WPBG-018

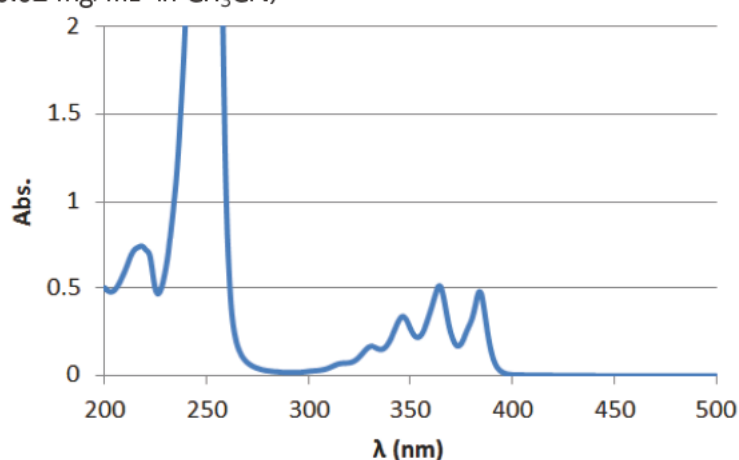
Chemical name | 9-Anthrylmethyl *N,N*-diethylcarbamate

Structural



Formula	C ₂₀ H ₂₁ NO ₂
Molecular weight	307.39
CAS No.	1228312-05-7
Melting point	72°C
TG-DTA	weight loss from 202°C
Appearance	light yellow - yellow crystals - powder
TSCA	—
EINECS	—

UV

(0.02 mg/mL in CH₃CN)

Absorption maximum

248 nm ($\epsilon=57000$)254 nm ($\epsilon=49400$)365 nm ($\epsilon=8800$)

Solubility

(g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
>50	>50	>50	>50	>50	>50	10	<0.5

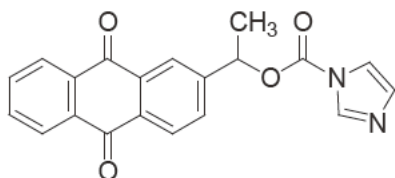
Characteristics

- Light absorption in long-wavelength region, and has excellent solubility.
- Shows high stability in different monomers.
- Generates diethylamine (b.p. =55°C) of secondary amine by light irradiation.
- Can be used as a sensitizer for WPBG-300 and WPBG-345.

WPBG-140

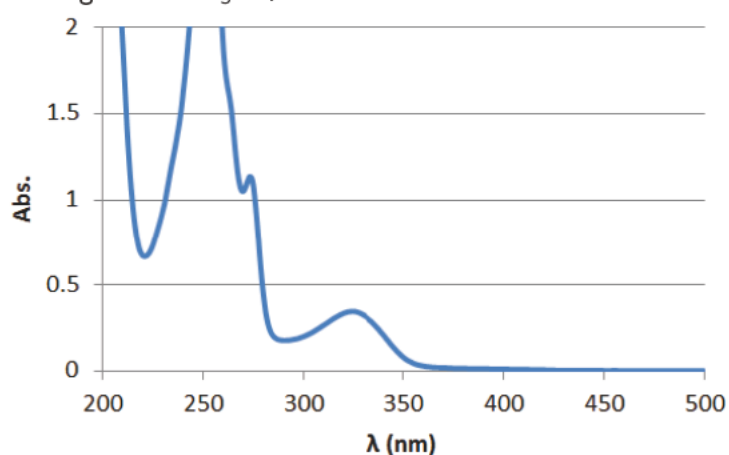
Chemical name | 1-(Anthraquinon-2-yl)ethyl imidazolecarboxylate

Structural



Formula	$C_{20}H_{14}N_2O_2$
Molecular weight	346.34
CAS No.	1418139-51-1
Melting point	124°C
TG-DTA	weight loss from 166°C
Appearance	pale yellow powder - mass
TSCA	—
EINECS	—

UV

(0.02 mg/mL in CH_3CN)

Absorption maximum

253 nm ($\epsilon=61400$)254 nm ($\epsilon=61200$)365 nm ($\epsilon=390$)

Solubility

(g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
14	11	1	<0.5	5	1	1	<0.5

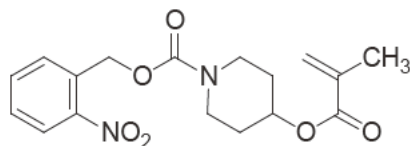
Characteristics

- Exhibits absorption region in the vicinity of 350 nm.
- Generates imidazole (m.p.=89-91°C, b.p.=256°C) by light irradiation
- Has radical polymerization initiating ability.

WPBG-165

Chemical name | (2-Nitrophenyl)methyl 4-(methacryloyloxy)piperidine-1-carboxylate

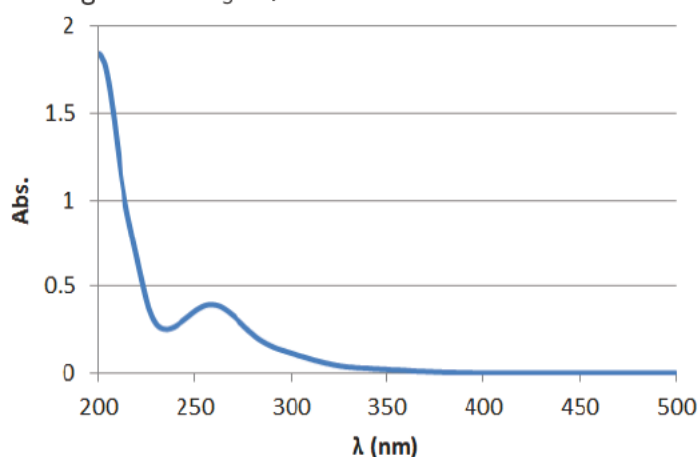
Structural



Formula	$C_{17}H_{20}N_2O_6$
Molecular weight	348.35
CAS No.	1292812-05-5
Melting point	55°C
TG-DTA	weight loss from 219°C
Appearance	white - light yellow powder
TSCA	—
EINECS	—

UV

(0.02 mg/mL in CH_3CN)



Absorption maximum

258 nm ($\epsilon=6400$)

254 nm ($\epsilon=6300$)

365 nm ($\epsilon=200$)

Solubility

(g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H_2O
>100	>100	>100	>100	10	10	10	<0.5

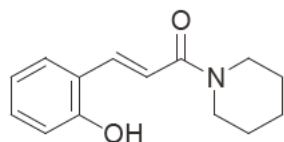
Characteristics

- Can introduce PBG into polymer by radical polymerization since it has a polymerizable methacrylic group.
- Has excellent solubility
- Generates 4-methacryloxy piperidine of secondary amine by light irradiation.

WPBG-027

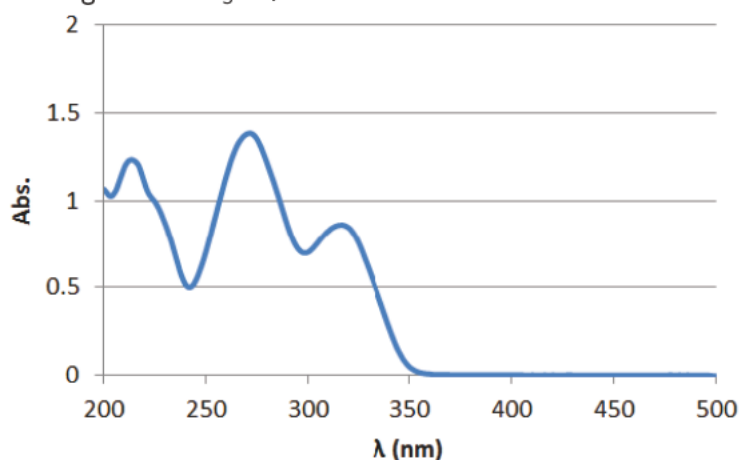
Chemical name | (*E*)-1-Piperidino-3-(2-hydroxyphenyl)-2-propen-1-one

Structural



Formula	C ₁₄ H ₁₇ NO ₂
Molecular weight	231.29
CAS No.	1203424-93-4
Melting point	232°C
TG-DTA	weight loss from 220°C
Appearance	White crystalline powder - mass
TSCA	—
EINECS	—

UV

(0.02 mg/mL in CH₃CN)

Absorption maximum

271 nm (ε=13500)

254 nm (ε=8700)

365 nm (ε=35)

Solubility

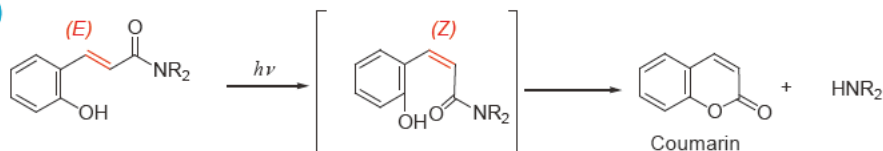
(g/solv. 100 g)

NMP	GBL	PGMEA	Acetone	Ethyl lactate	PGME	Methanol	H ₂ O
8	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5

Characteristics

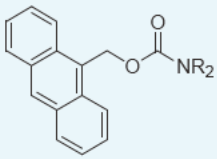

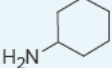
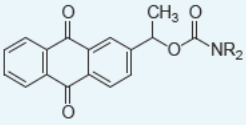
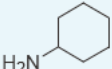
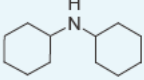
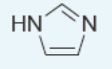
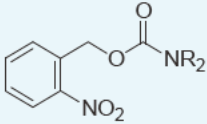
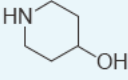
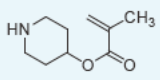
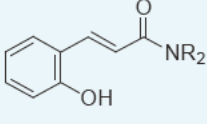
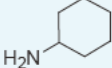

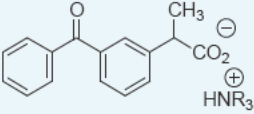
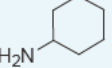
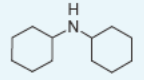
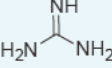
- Generates piperidine (b.p. = 106°C) of secondary amine by light irradiation.
- Does not generate carbon dioxide gas at the time of base generation.
- Shows high heat stability in different monomers.
- Soluble in strong alkali due to its phenolic hydroxyl functionality.

Mechanism of base generation





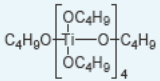
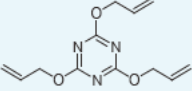
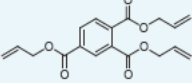
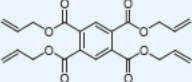
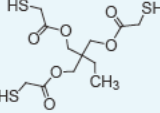
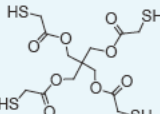
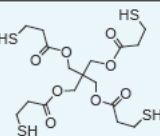
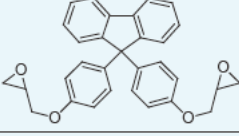
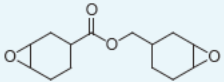
Reference


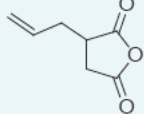
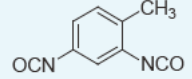
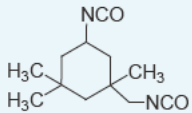
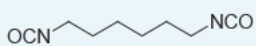
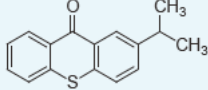
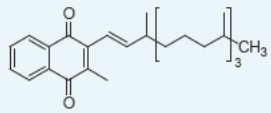
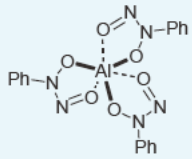
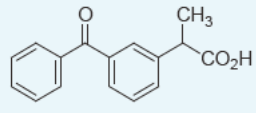
K. Arimitsu., *et al.*, *Polymer Preprints, Japan*, 2007, 56, 4263.

Main Structure	Generated Base	Product Name	Product code	Packaging
		WPBG-015 9-Anthrylmethyl Piperidine-1-carboxylate	359-33631	1 g
			355-33633	5 g
	HNEt ₂	WPBG-018 9-Anthrylmethyl <i>N,N</i> -diethylcarbamate	356-33641	1 g
			352-33643	5 g
		WPBG-041 9-Anthrylmethyl <i>N</i> -cyclohexylcarbamate	353-33651	1 g
			359-33653	5 g
		WPBG-174 1-(Anthraquinon-2-yl)ethyl <i>N</i> -cyclohexylcarbamate	351-33691	1 g
			357-33693	5 g
		WPBG-166 1-(Anthraquinon-2-yl)ethyl <i>N,N</i> -dicyclohexylcarbamate	354-33681	1 g
			350-33683	5 g
		WPBG-140 1-(Anthraquinon-2-yl)ethyl imidazole-1-carboxylate	357-33671	1 g
			353-33673	5 g
		WPBG-158 (2-Nitrophenyl)methyl 4-hydroxypiperidine-1-carboxylate	358-33721	1 g
			354-33723	5 g
		WPBG-165 (2-Nitrophenyl)methyl 4-(methacryloyloxy)piperidine-1-carboxylate	355-33731	1 g
			351-33733	5 g
		WPBG-025 (<i>E</i>)- <i>N</i> -Cyclohexyl-3-(2-hydroxyphenyl)acrylamide	354-33701	1 g
			350-33703	5 g
		WPBG-027 (<i>E</i>)-1-Piperidino-3-(2-hydroxyphenyl)-2-propen-1-one	351-33711	1 g
			357-33713	5 g
		WPBG-168 Cyclohexylammonium 2-(3-benzoylphenyl)propionate	359-33751	1 g
			355-33753	5 g
		WPBG-167 Dicyclohexylammonium 2-(3-benzoylphenyl)propionate	356-33761	1 g
			352-33763	5 g
		WPBG-082 Guanidinium 2-(3-benzoylphenyl)propionate	352-33741	1 g
			358-33743	5 g

List of PBG-related Items

2016.1.27

	Structural	Product Name	Product code	Packaging
Metal alkoxide	$\text{Si}(\text{OEt})_4$	Tetraethyl Orthosilicate	053-03476	500 mL
		3-Glycidoxypropyltrimethoxysilane	302-60432	25 g
		[2-(3,4-Epoxy)cyclohexyl]ethyltrimethoxysilane	321-91252	25 g
			329-91253	100 g
	$\text{OCN}-\text{CH}_2\text{CH}_2\text{CH}_2-\text{Si}(\text{OEt})_3$	3-(Triethoxysilyl)propyl Isocyanate	324-91242	25 g
			322-91243	100 g
			$\text{Ti}(\text{O}/\text{Pr})_4$	Titanium Tetraisopropoxide
			207-08176	500 mL
			$\text{Ti}(\text{OC}_4\text{H}_9)_4$	Titanium(IV) Tetrabutoxide
		Titanium(IV) Tetrabutoxide, Tetramer	205-09772	25 mL
			209-09775	500 mL
	$\text{Zr}(\text{O}t\text{-Bu})_4$	Zirconium(IV) <i>t</i> -Butoxide	353-13491	5 g
Polyfunctional allyl		2,4,6-Tris(allyloxy)-1,3,5-triazine	201-02292	25 g
			205-02295	500 g
		TRIAM®-705	909-40246	500 g
	TRIAM®-805	863-43710	500 g	
Polyfunctional thiol		Trimethylolpropane Tris(mercaptoacetate)	327-21642	25 g
			321-21645	500 g
		Pentaerythritol Tetrakis(mercaptoacetate)	326-21612	25 g
			320-21615	500 g
		Pentaerythritol Tetrakis(3-mercaptopropionate)	329-21722	25 g
			323-21725	500 g
Polyfunctional epoxy		9,9-Bis[4-(glycidyloxy)phenyl]fluorene	325-24421	10 g
			321-24423	100 g
		3,4-Epoxy cyclohexylmethyl	326-64072	25 g
			3,4-Epoxy cyclohexanecarboxylate	320-64075

Acid anhydride		Methyl-5-norbornene-2,3-dicarboxylic Anhydride	134-05951	200 g
			136-05955	500 g
		Allylsuccinic Anhydride	015-20331	5 g
			013-20332	25 g
Isocyanate		Toluene 2,4-Diisocyanate	205-04892	25 g
			209-04895	500 g
		3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate (mixture of isomers)	090-03022	25 mL
			094-03025	500 mL
		Hexamethylene Diisocyanate	082-02822	25 g
			086-02825	500 g
Sensitizer		2-Isopropylthioxanthone	352-28932	25 g
			350-28933	100 g
		Vitamin K ₁	221-00371	1 g
			227-00373	5 g
Polymerization inhibitor		N-Nitroso-N-phenylhydroxylamine Aluminium Salt	143-04562	25 g
			147-04565	500 g
Carboxylic acid		Ketoprofen	115-00381	5 g
			113-00382	25 g

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