DMI™ is an aprotic solvent with high polarity.

DMI™

1,3-Dimethyl-2-Imidazolidinone

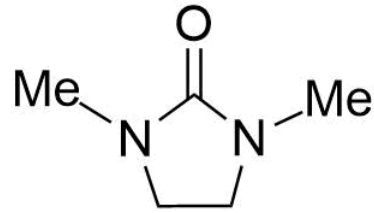
I Product Overveiw

DMI™ is an aprotic solvent with high polarity. DMI™ is used in a wide range of fields for its excellent dissolving power, stability, and high quality

【Substance】

Chemical Name	1,3-Dimethyl-2-Imidazolidinone
Synonyms	DMEU Dimethylethyleneurea
CAS No.	80-73-9

【Structural Formula】



【Regulatory Information】

United States	TSCA:	On this inventory, or in compliance with the inventory.
European Union	REACH:	Contact us for information.
Canada	DSL: NDSL:	Not in compliance with the inventory.
Australia	AICS:	On this inventory, or in compliance with the inventory.

【Characteristic】

Physical properties

DMI™ is easy to handle since boiling point and flash point are high, and freezing point is low.
(Boiling point 222℃、Flash point 120℃(open cup)/ 95℃(closed cup)、Melting point 7.5℃)

Stability

Compared to general aprotic polar solvents, DMI™ is stable even in the presence of acids and alkalis.
DMI™ has excellent resistance to acids and alkalis at high temperature

Solubility

Due to high dielectric constant and dipole moment, DMI™ exhibits high solubility in various inorganic and organic compounds.

【 Applications 】

Reaction solvents (for synthesis of pharmaceuticals, agricultural chemicals, and polymers), detergents, additives, solvents, surface treatment agents etc.

【Specification 】

Items	Specification	Test method
APPEARANCE	COLORLESS LIQUID	MCI method
COLOR (APHA)	≦50	MCI method
PURITY (GC%)	≧98.0	MCI method
REFRACTIVE INDEX (n_D^{25})	1.468 -1.473	MCI method
MOISTURE (wt%)	≦0.1	MCI method

【Packing】

Container	Net weight
Iron Can	18KG
Iron Drum	200KG

II Physical Properties

1. Physical Constants

Items	Units	Physical constants
Molecular weight	—	114.14
Boiling point	(℃)	222 (760mmHg)
Melting point	(℃)	7.5
Specific gravity	(d_4^{20})	1.06
Refractive index[1)]	(n_D^{25})	1.471
Kinetic viscosity[1)]	$(mm^2/_S)$	1.95 (20℃) 1.43 (40℃)
Surface tension	(mN/m)	41 (20℃)
Specific heat	(J/g·℃)	1.80 (adiabatic continuity method, 20℃)
Heat conductivity	(kJ/hr·m·℃)	0.62 (thermic rays method、25℃)
Vaporization latent heat	(kJ/mol)	51.9 (=454.7J/g)
Flash point	(℃)	120 (Cleveland open method) 95 (Pensky-Martens close method)
Dipole moment[1)]	(D)	4.05～4.09
Dielectric constant[1)]	(F/m)	37.60 (25℃、1MHz)

1) J. Chem. Eng. Data 21, 150 (‘76)

2. Physical constants compared with other solvents

DMI™ has high values of dielectric constant and dipole moment, and solubility and solvation effect are high compared to similar solvents

	Boiling point (℃)	Melting point (℃)	Dielectric constant[2)] (F/m)	Dipole moment(D)	Flash point (℃)	Viscosity[3)] (mPa·s)
DMI™	222	7.5	**37.6**	4.05 - **4.09**	120	1.94
DMF	153	-61	**37.6**	3.86	53	0.92
DMAC	165.5	-20	**37.8**	3.72	66	0.92
NMP	220	-24	32	**4.09**	81.3	1.67

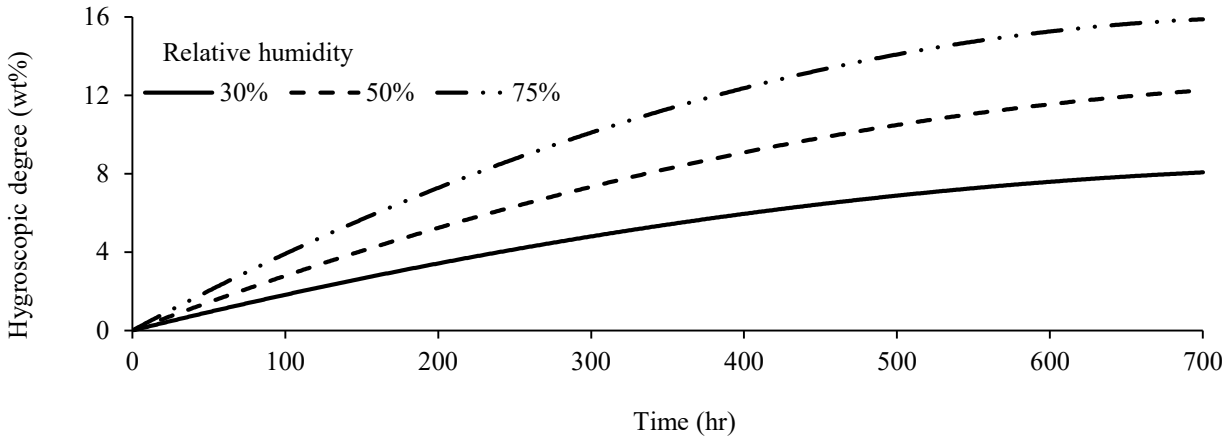
2) 25℃, 1MHz
3) DMI ™ 25℃, Others 20℃

3. Temperature dependency of dielectric constant, viscosity, density and refractive index

Temperature (℃)	Dielectric constant[4] (F/m)	Absolute viscosity (mPa·s)	Density (kg/m^3)	Refractive index (n_D^{25})
25	37.60	1.944	1,052	1.471
35	35.97	1.633	1,043	1.466
45	34.43	1.393	1,034	1.462
55	32.96	1.204	1,025	-
75	30.35	0.938	1,008	-
100	27.42	0.720	986	-

4) 25℃, 1MHz

4. Rate of moisture adsorption

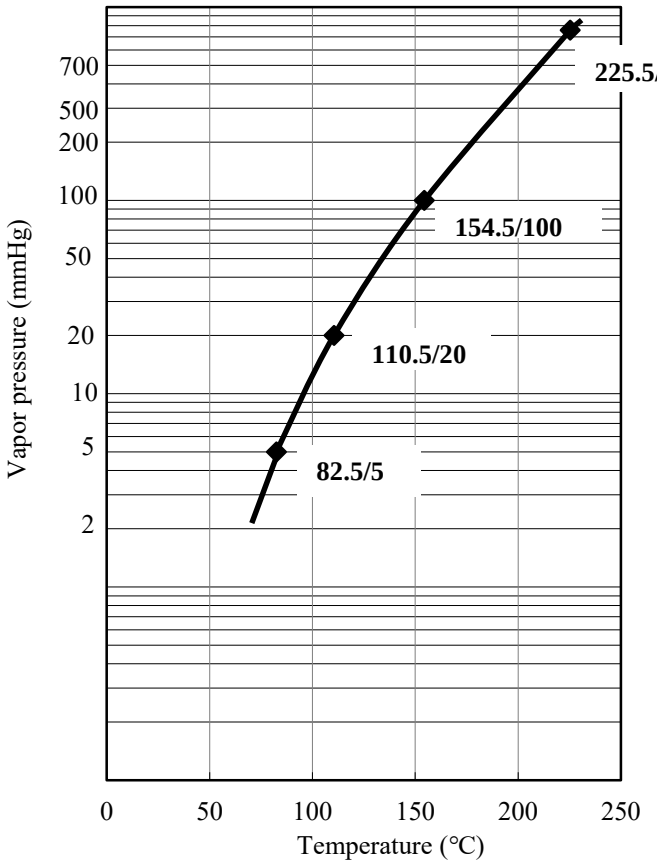


5. Change of water content with drying agent

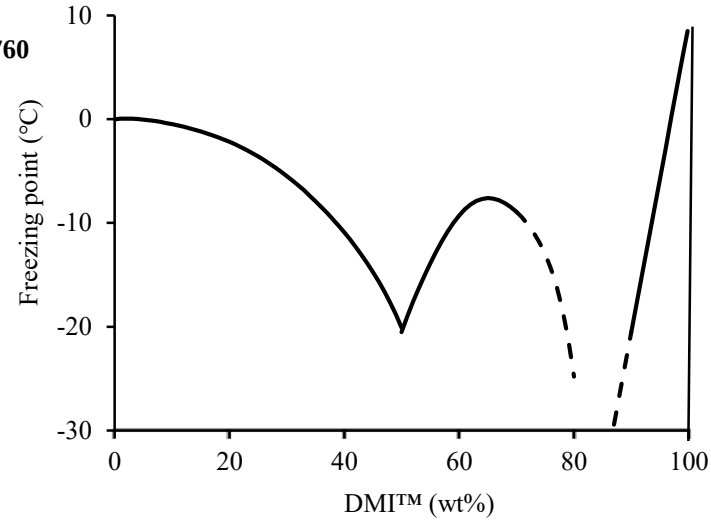
Drying agent	Water content(ppm)			
	Initial	After 2.5hr	After 68hr	After 116hr
KOH	1,523	1,624	1,683	2,211
CaH_2	1,523	1,260	216	96
Zeolite A-3 Pellet1.5mmΦ	1,523	200	14	6

Drying agent (10g) was added in DMI™ (50g). After shaking with hand, the water content was measured by the Karl-Fischer Method.

6. Vapor pressure curve



7. Freezing point of the mixture with water



8.Solubility of inorganic compounds

Inorg.Compd.	g/100g	(°C)	Inorg.Compd.	g/100g	(°C)
$AgNO_3$	50	(60)	LiCl	50	(70)
$AlCl_3$	35	(20)	$NaBH_4$	11.4	(25)
$CaCl_2$	5	(20)	NaBr	3.2	(20)
CaF_2	0.02	(20)	NaCl	0.05	(20)
CH_3ONa	0.02	(20)	NaCN	0.02	(20)
$CuCl_2$	4	(20)	Na_2CO_3	＜0.01	(20)
$FeCl_3$	＞50	(20)	NaI	＞200	(20)
I_2	＞150	(20)	NaOH	＜0.1	(25)
KCN	0.03	(20)	PCl_3	＞50	(20)
K_2CO_3	＜0.01	(20)	P_2O_5	70	(20)
KI	30	(60)	$Mg(ClO_4)_2$	＞50	(60)
KOH	＜0.1	(25)	S	11	(100)
KSCN	50	(80)	$ZnCl_2$	50	(60)
LiBr	9.3	(20)	ZnO	5	(20)

9. Solubility of inorganic compounds

Inorg.Compd.	g/100g (℃)		
	DMI™	DMF	NMP
$CaCl_2$	5 (20)	0.5 (r.t.)	–
$FeCl_3$	＞50 (20)	＞20 (r.t.)	–
I_2	＞150 (20)	＞25 (r.t.)	–
KCN	0.03 (20)	0.22 (r.t.)	–
K_2CO_3	＜0.01 (20)	0.05 (r.t.)	–
KOH	＜0.1 (25)	0.1 (r.t.)	–
LiBr	9.3 (20)	–	25.5 (25)
$NaBH_4$	11.4 (25)	25.5 (r.t.)	
NaBr	3.2 (20)	–	5.5 (25)
NaCl	0.05 (20)	＜0.05 (r.t.)	0.02 (25)
NaCN	0.02 (20)	0.76 (r.t.)	–
Na_2CO_3	＜0.01 (20)	＜0.05 (r.t.)	–
NaI	＞200 (20)	14.4 (r.t.)	28.8 (25)

10. Solubility of organic compounds (at room temperature)

Org. Compd.	Solubility
Petroleum Benzine	insoluble
Cyclohexane	insoluble
Decalin	soluble
Xylene	soluble
Tetralin	soluble
Chloroform	soluble
Trichloroethylene	soluble
Methanol	soluble
Isopropyl alcohol	soluble
n-Octyl alcohol	soluble
Ethylene glycol	soluble
Ethyl ether	soluble
Tetrahydrofuran	soluble

Org. Compd.	Solubility
Acetone	soluble
Acetic acid	soluble
Acetonitrile	soluble
Benzonitrile	soluble
Dimethylformamide	soluble
Ethyl acetate	soluble
Methyl benzoate	soluble
Aniline	soluble
Pyridine	soluble
Quinoline	soluble
Crbon disulfide	soluble
Sulfolane	soluble
Nitrobenzene	soluble
Nitromethane	soluble

11. Solubility of resins

Chemical name	Solubility% (℃)	
Epoxy resin	＞100	(20)
Acrylic styrene resin	＞45	(20)
Polystyrene	＞45	(20)
Vinylidene fluoride	＞30	(20)
Phenol-formaldehyde resin	＞20	(20)
Polyvinylchloride	＞20	(20)
Nylon	＞5	(160)
Polyvinylalcohol	＞5	(80)
Polyacrylonitrile	＞5	(70)
Ultem	＞3	(120)

Chemical name	Solubility% (℃)	
Polysulfone	＞3	(20)
Polyethersulfone	＞3	(20)
Polymethylmethacrylate	＞3	(20)
Polyurethane	＞1	(70)
U-polymer	＞1	(20)
Noryl	＞1	(20)
Polyacrylamide	＜1	(120)
Polyetheretherketone	＜1	(120)
Polyphenylenesulfide	＜1	(120)
Polycarbonate	swollen	(20)
Polytetrafluoroethylene	insoluble	
Polyethylene	Insoluble	

12. Explosibility

Lower explosion limit 1.3%
Upper explosion limit 8.4%

13. Solubility parameter

A solubility parameter is calculated as follows:

$$\delta=\sqrt{\frac{\triangle H-RT}{(M/d/10^3)}} \quad (J/cm^3)^{1/2} \text{-①}$$

where
△H= heat of vaporization(J/mol)
R=gas constant (J/K･mol)
T=absolute temperature (K)
M=molar weight (g/mol)
d=density (Kg/m^3)

when the following values are substituted in ①,

△H=51,882 (J/mol)
R=8.315 (J/K･mol)
T=298 (K)
M=114.14 (g/mol)
d=1,052 (Kg/m^3)

The solubility parameter of DMI^{TM} is obtained as follows:

$$\delta=\sqrt{\frac{51{,}882-(8.315)\times(298)}{(114.14/1{,}052/10^3)}}=\sqrt{455.3}=21.3(J/cm^3)^{1/2}$$

14. Distribution coefficients between organic compounds and water

Org. Compd.	Distribution coefficient (27℃～30℃)
Chloroform	2.5
Dichloromethane	2.5
1,2-Dichloroethane	0.77
1,1,2-Trichlorethylene	0.26
Benzene	0.22
Toluene	0.14
1,1,2-Trichloroethane	0.12
Diethylether	0.06

Distribution coefficient = conc.of DMI^{TM} in org.layer/ conc.of DMI^{TM} in water layer

III Chemical properties

Stability to acids and alkalines

DMI™ can be used for a wide variety of uses because DMI™ has higher heat stability in the presence of acids and alkalines than general aprotic polar solvents.

◆Stability in acids (in a stream of N_2)

	DMI™ Residual ratio (%)		NMP Residual ratio (%)	
	0hr	12hr	0hr	12hr
Flake NaOH(3g)/ DMI™ or NMP (30g), 200℃	100	100	100	69
Powder K_2CO_3(3g)/ DMI™ or NMP(30g), 200℃	100	100	100	86
10% NaOH(3g)/ DMI™ or NMP (7.5g), 100℃	100	100	100	29

◆Stability in alkalines (in a stream of N_2)

	DMI™ Residual ratio (%)		NMP Residual ratio (%)	
	0hr	12hr	0hr	12hr
50% Sulfuric acid, (15g)/ DMI™ or NMP (30g), 100℃	100	100	100	77

IV Example of applications

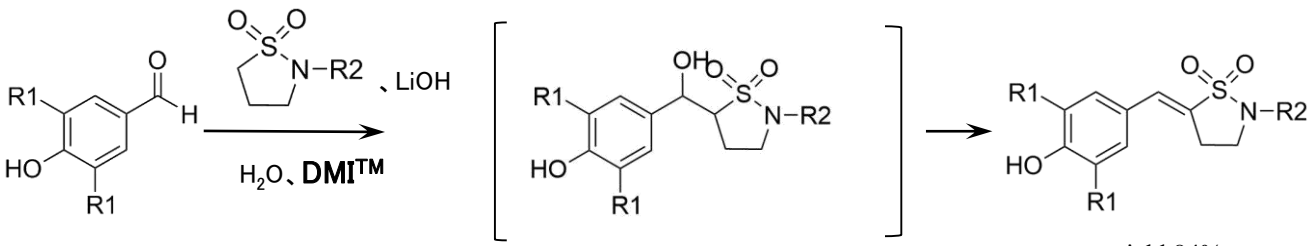
1. Solvent for reaction

With its high dielectric constant and solvation effect, DMI™ accelerates anionic nucleophilic reactions, and reactions that place with solvation of cation.
DMI™ is thermally and chemically stable with excellent dissolving power for organic and inorganic compounds.
Since DMI™ is extremely useful as a reaction solvent, it is used in various reactions to synthesize medical drugs and pesticides.

◆*Pharmaceutical synthesis*

▪Aldol condensation

As a reaction solvent in the production of benzylidene derivatives that are used as anti-inflammatory agents.

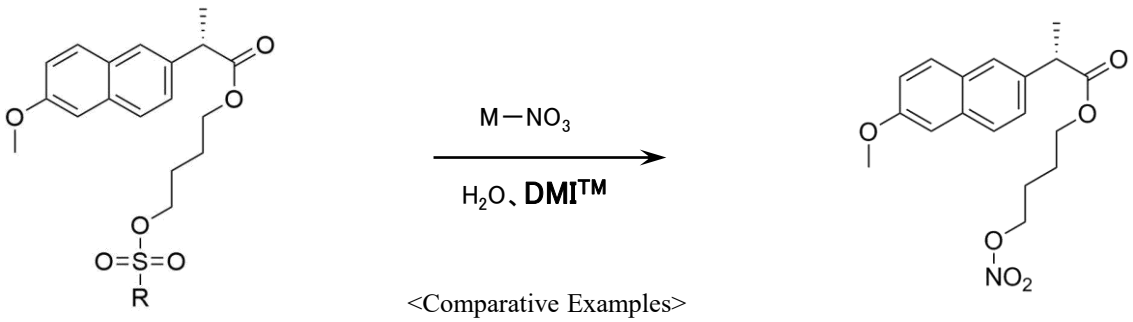


yield 84%

WO2004089921A

▪Nitric acid esterification

As a reaction solvent in the production of (S)-naproxen-4-nitroxybutyl ester used as anti-inflammatory agents, and analgesics.



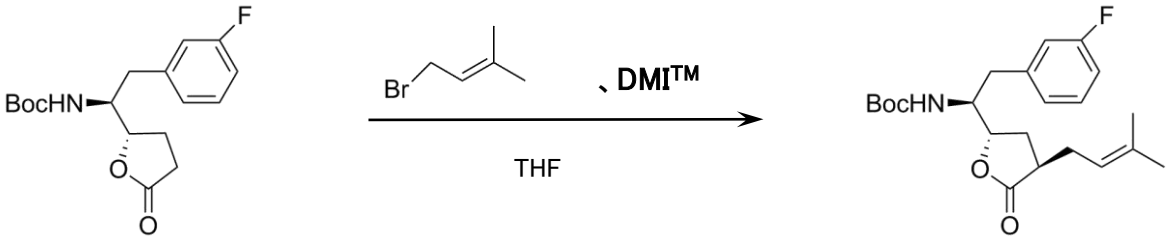
<Comparative Examples>
Tetramethylurea 89%
Sulfolane 74%
NMP 73%

yield 99%

WO2003045896A / JP2005510557T2

▪Alkylation

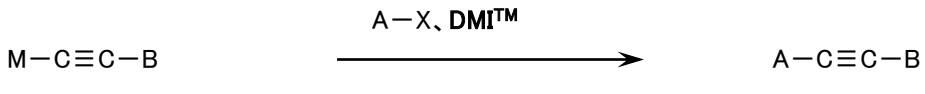
(1) As a reaction additive in the production of alkyl compounds of γ-butyrolactone.



yield 90～92%

Organic Process Research & Development, (2001),5(6), p609-611

(2) As a reaction additive in the production of substituted acetylene compounds used as pharmaceutical intermediates.



yield 94%

A : a saturated or unsaturated aliphatic hydrocarbon residue of 1 to 20 carbon atoms
X : a halogen atom or an arylsulfonyloxy group
M : an alkali metal
B : H、a hydrocarbon residue or －C≡C－M

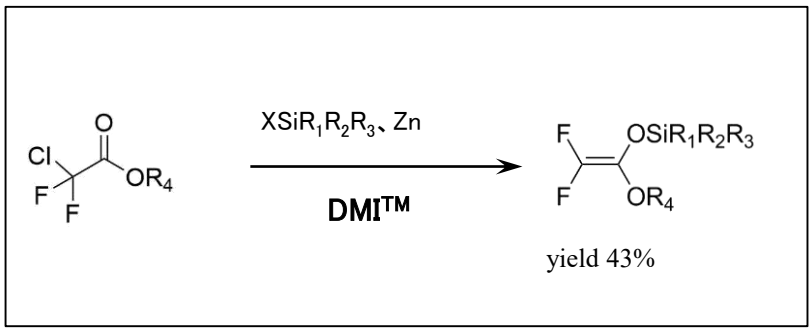
EP284237A1

<Comparative Examples >

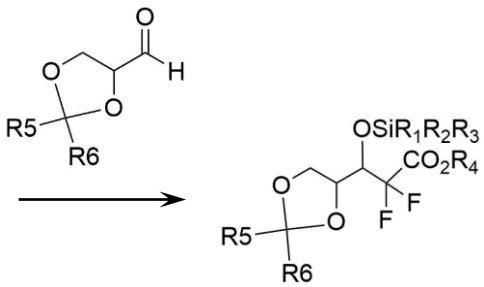
Ethylenediamine	66%
Tetramethylurea	62%
DMF	24%
NMP	19%
DMSO	18%

▪Silyl etherification

As a reaction solvent in the production of silyl ether compound used as pharmaceutical intermediates.



yield 43%



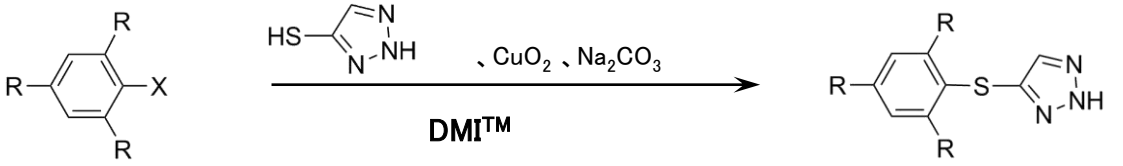
<Comparative Examples>

NMP	4%
Acetonitrile	1.2%
DMF	N.D.

US561895A / JP3615253B2

◆*Agricultural synthesis*

・As a reaction solvent in the production of triazole derivative used as an herbicide.

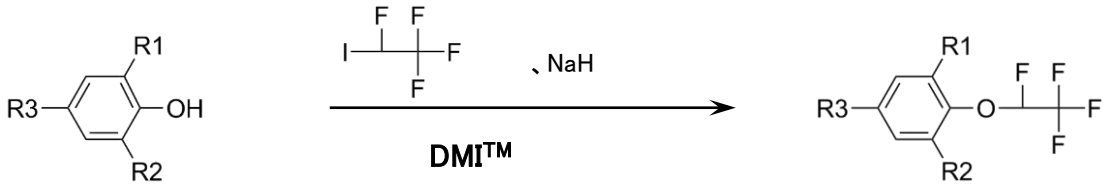


yield 71%

<Comparative Examples >
DMF trace
DMSC trace
DMAC trace

EP718291A / JP08176117A

・As a reaction solvent to produce tetrafluoroethoxybenzenes used as intermediates for germicides, antibacterial agents, insecticides, and herbicides.



(R1、R2:H、F R3:Halogen、Aldehyde、or Mesogenic group)

DE4408151A1

◆*Polymer synthesis*

DMI™ improves the reactivity with its excellent solubility, cation solvation, and suppresses side reactions because of its high stability at high temperatures and in the presence of alkalis.

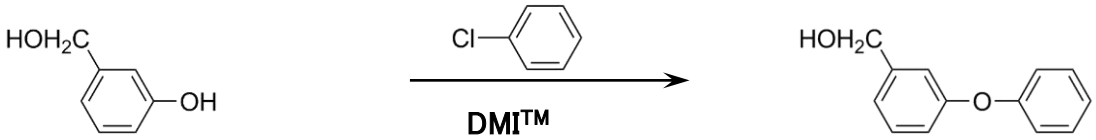
- In the production of polyamides and polyimides, DMI™ accelerates the formation of amide and imide groups to produce high molecular weight polymers.[1)]
- Polymers suitable for electronic parts with less ionic impurities can be obtained in the production process of polyphenylene sulfide.[2)]
- DMI™ can suppress side reactions in the production process of polyethersulfone to produce high quality polymers.[3)]
- DMI™ treatment during film formation of polyimide, stretching of polyether ketone film, and production of polysulfone membrane produces uniform and excellent quality products.[4)]

1)JP63108027A, JP 05140308A
2)JP63268740A
3)JP0586186A
4)JP61195130A, JP0313314A, JP6219209A

◆*Other reactions*

▪ Phenyl ethers

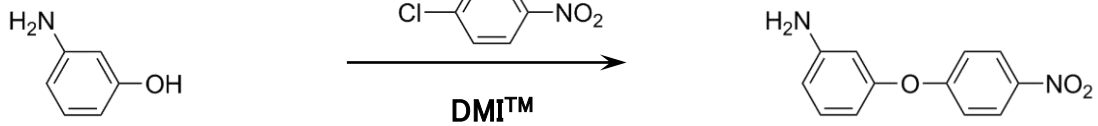
(1)



JP61257938A

yield 93%

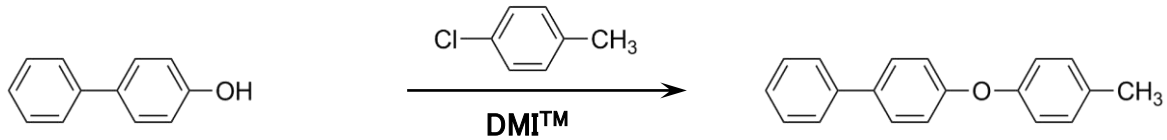
(2)



JP6317852A

yield 97%

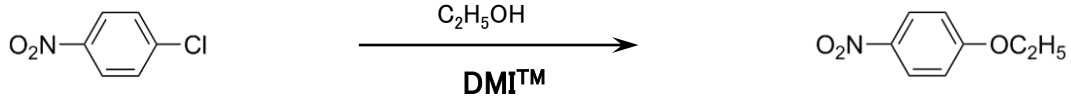
(3)



JP01160935A

yield 92%

(4)

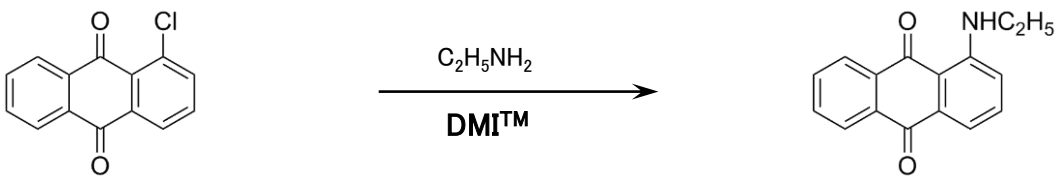


JP03232841A

yield 97%

▪ Amines

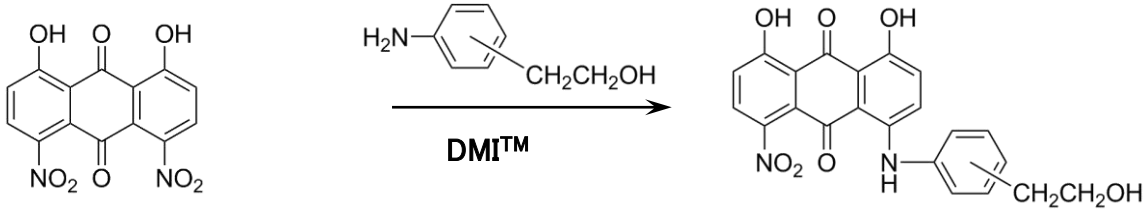
(1)



JP06247912A

yield 97%

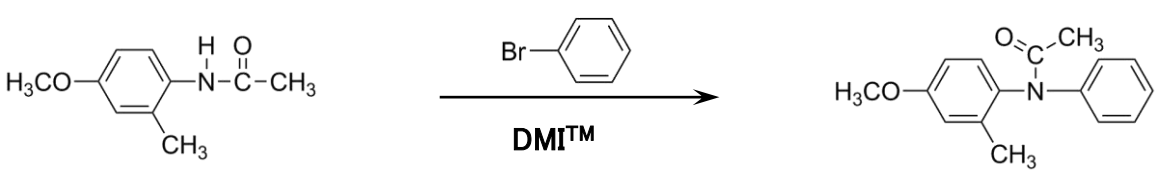
(2)



JP05170713A

yield 91%

(3)

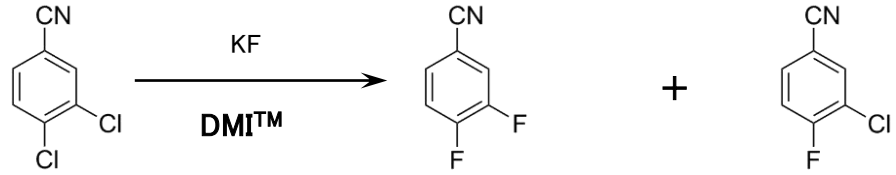


JP63165350A

yield 95%

▪ Fluorobenzenes

(1)

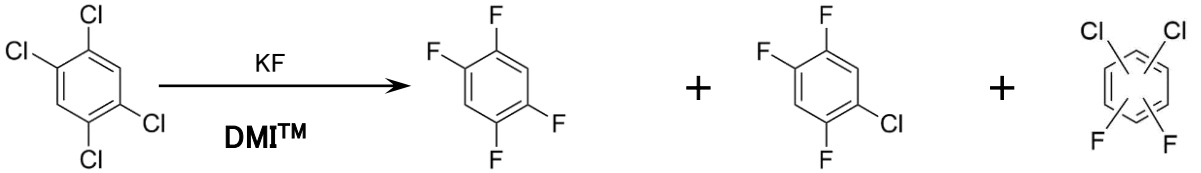


A yield 65%　　B yield 23%

<Comparative Examples>
DMPU A=47%
B=30%
$TMSO_2$ A=38%
B=43%

JP03145449A

(2)



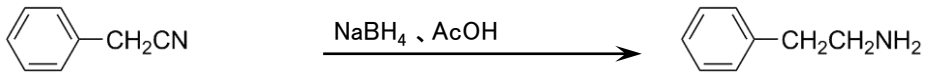
<Comparative Example>
NMP A=N.D.
B=3.3%
C=6.2%

A yield 12%　　B yield 48%　　C yield 23%

JP05117181A

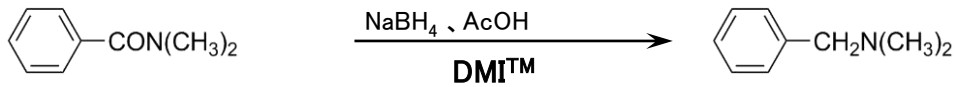
▪ Reduction

(1)



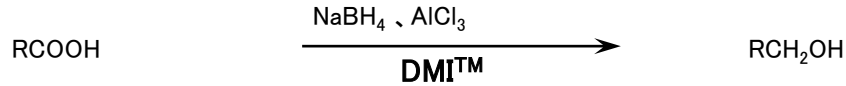
yield 70%

(2)



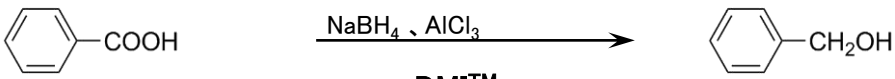
yield 90%

(3)



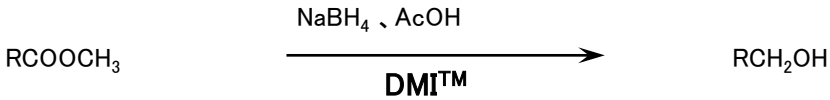
yield 78%

(4)



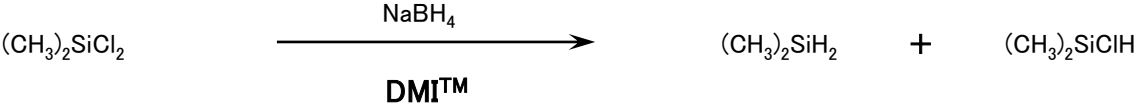
yield 78%

(5)



yield 99%

(6)

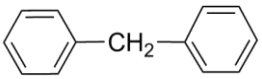


A yield 10%　　B yield 49%

JP54144301A

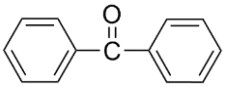
・Oxydation

(1)



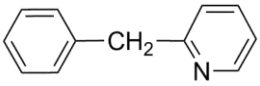
O_2 、NaOH

DMI™



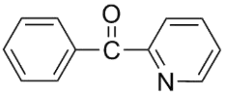
yield 88%

(2)



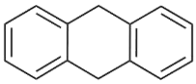
O_2 、NaOH

DMI™



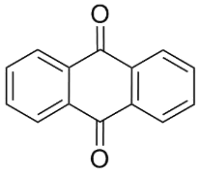
yield 82%

(3)



O_2 、NaOH

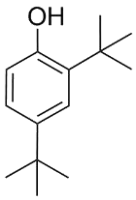
DMI™



JP54144348A

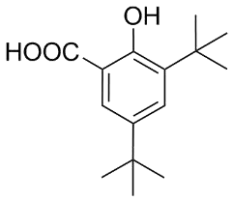
yield 88%

・Kolbe-Schmitt reaction



CO_2 、KOH

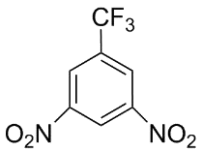
DMI™



JP0390047A

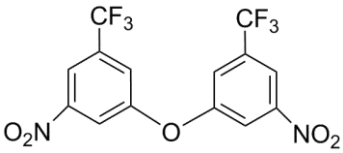
yield 92%

・Self-condensation



$NaNO_2$

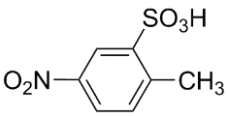
DMI™



JP05230012A

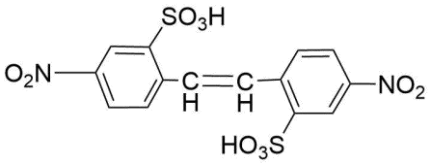
yield 60%

・Dimerization



NaOH

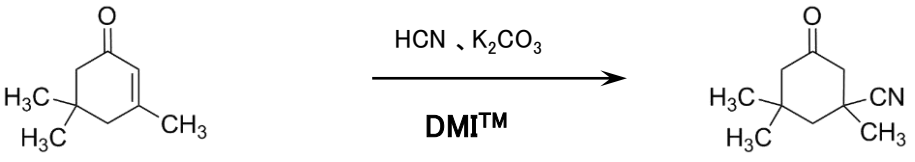
DMI™



JP05178796A

yield 90%

・Addition reaction

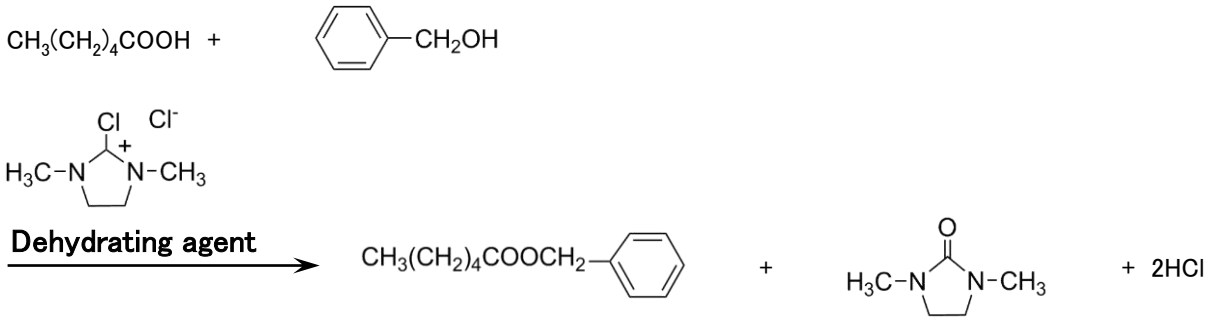


JP04164057A

yield 83%

・Dehydrating agent

DMI™ reacts with halogenating reagents such as phosgene, oxalyl chloride, and is effective as a dehydrating agent.



yield 96%

JP6245223A

2. Detergents

DMI™ has strong dissolving power and is used in detergents such as paint peeling agents and photoresist stripping agents.[5)]

5)JP0715111A, JP06228591A

◆*Paint peeling agents*

A patent example for DMI™ used in paint peeling agents of acrylic, melamine, urethane type resins, which have sufficient paint removability and excellent workability.

The results after the evaluation test is shown in the table with number of changes for each of the following, ◎ when changes are observed in the coating and primer resin; O, when the primer resin peels off by disintegration or swelling; Δ when peeling off is observed by partial dissolution or disintegration or swelling; X when no changes are observed (5 test samples were used)

Detergents	Composition (wt%)	Temperature (℃)	Results			
			◎	○	△	×
DMI™/EtOH	90/10	50～100	5			
Methylene Chloride	100	40			3	2
DMF	100	50～100			3	2
DMSO	100	50～100			4	1

※Acrylic curable paint with melamine coated on parts of polyolefin resin with primer
(Coating I and coating II have different chemical compositions for the coating and primer resins.)

6）JP2924323B2

◆*Photoresist Stripping Agents*

A patent example in which DMI™ has been used for photoresist stripping agents that are not corrosive to silver and silver alloys and has high peelability for photoresist and photoresist deteriorated layers[7)]

Photoresist Stripping Agents	Composition (mass%)	Results		
		Photoresist Peelability	Photoresist alteration layer Peelability	Corrosive to silver alloys
DMI™/2-(2-Aminoethoxy)ethanol	70/30	◎	◎	◎
DMI™/Monoethanolamine	70/30	◎	◎	×
DMI™/Triethanolamine	70/30	×	×	◎
DMI™/N,N-Diethanolamine	70/30	○	×	◎
DMI™/2-(2-minoethoxy)ethanol/Water	60/30/10	◎	×	×

※ Peelability:◎＝ Eliminable,○＝Slight remaining,× ＝ not eliminable
※ Corrosive :◎＝Remain the same,○＝Discolored parts occur,
× ＝ Discolored ・gloss level variation・stripped membranes parts occur

【Test Method】
The substrate used for evaluation was subject to dry etching and then immersed in a photoresist stripping agent at 70℃ for 10 minutes, and the peelability was evaluated using optical and electron microscopes.

Silver alloy corrosivity: A silver alloy formed on a glass substrate was immersed in a photoresist stripping agent at 70℃ for 10 minutes and evaluated for corrosivity using optical and electron microscopes.

7) WO2005/022268A1

3. Additives

DMI™ is used as an additive for adhesives, rubber processing aids, and electrolytes.

◆*Adhesives*

A patent example in which proper shape is retained, bonding duration is retained without decreasing the initial tack, has excellent and powerful adhesiveness that even bonds with coated paper for which adhesion is difficult, and used in the stick adhesive that has polyvinyl pyrrolidone as the main component.[8)]

	Example1	Example2	Example3
Adhesive ingredient[a)]	95%	95%	95%
Additive	DMI™ 5%	ε-Caprolactam 5%	None
Bonding strength test result[b)]	100%	90%	30%
Hardness test result[c)]	1.01	1.51	0.98

a)Adhesive composition: 27% of polyvinyl pyrrolidone, 8% of sodium stearate, 50% of water, and 10% of glycerin

b)Bonding strength test: Breaking rate of paper when high quality papers are stuck together and peeled after 3 days

c)Hardness: Penetration distance (mm) by a 12.5 g needle in 10 seconds. Smaller the penetration distance, greater the hardness

8)JP11189757A

◆*Rubber Processing Aids*

A patent example of use in a modifying agent of rubber processing aids that can avoid deterioration of rebound resilience due to addition of processing aids, and deterioration in processability due to dispersion of carbon black. Evaluation of extrusion processability using a rubber composition according to the ASTM D2230-77A method

Denaturant	Weight average molecular weight of liquid rubber	Additive amount of liquid rubber[a)]	60°C Repulsive[b)]	Wetskid resistance[c)]	Extrusion processability
DMI™	6,000	10	59	61	16
None	6,000	10	55	58	12

a) The amount of liquid rubber added is based on 100 g of SBR

b) The test specimen exposed to the atmosphere at 60°C was measured according to JIS K-6301

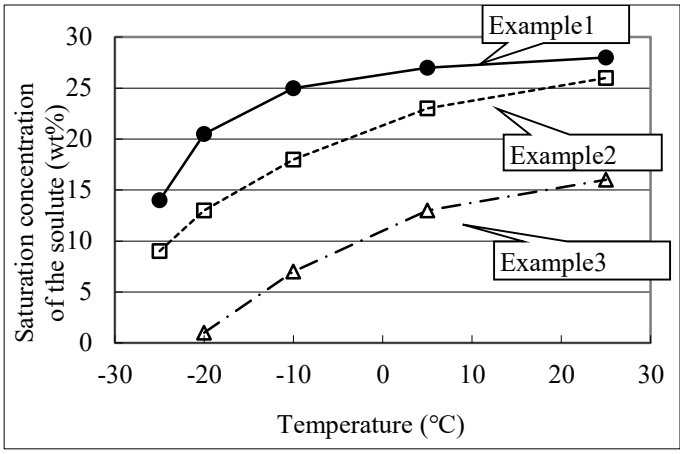
c) Measured using a portable skid tester on the road surface of ASTME-303-74 specifications at 23°C (manufactured by Stanley UK)

9) JP03281645A

◆*Electrolytes*

A patent example showing high specific conductivity and thermal stability, used as a solute precipitation inhibitor for electrolyte in which the solute of diazabicycloalkene carboxylate salt does not precipitate even at low temperatures[10)]

	Electrolyte composition(wt%)	Specific conductivity (30℃,ms/cm)	
		Initial	After the heat treatment
Example1	Solute(25) γ－Butyrolactone(70) DMI™(5)	7.1	7.2
Example2	Solute(20) γ－Butyrolactone(65) Ethylene glycol(15)	7.0	4.9
Example3	Solute(10) γ－Butyrolactone(90)	4.5	4.5



Solute：Phthalic acid mono-1,5-Diazabicyclo[4.3.0]non-5-ene
The heat treatment：150℃，10 hours

10)JP097895A

4. Solvent

When DMI™ is used as a solvent in the ink of inkjet printers, print density, drying resistance, and storage stability of the ink are known to improve.[11)]

11)JP04339873A, JP06172690A

5. Surface treatment agent

When the surface of the Teflon, a fluorine resin, is treated using a solution (etching agent) prepared by dissolving sodium, potassium, and lithium metal polyallyl complex dispersion is dissolved in DMI™, the bonding strength of epoxy resin adhesive improves[12)]

12)JP5484501A

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For the detailed safety information, please refer to Materials Safety Data sheet of DMI™.

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