

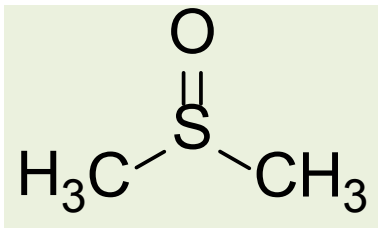
# TORAY

Innovation by Chemistry

Toray Fine Chemicals Co., Ltd.

## TFC's proposal to settle your concerns of **REACH regulation, Solubility, Hazard and Toxicity.**

We suggest the mixed solvent with appropriate ratio of each component by theory calculation and actual survey of HSP (Hansen solubility parameter).

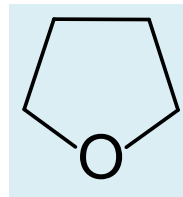


**DMSO**

[Dimethyl Sulfoxide]

CAS RN<sup>®</sup> : 67-68-5

EC Number : 200-664-3



**THF**

[Tetrahydrofuran]

CAS RN<sup>®</sup> : 109-99-9

EC Number : 203-726-8

# HSP (Hansen Solubility Parameter)

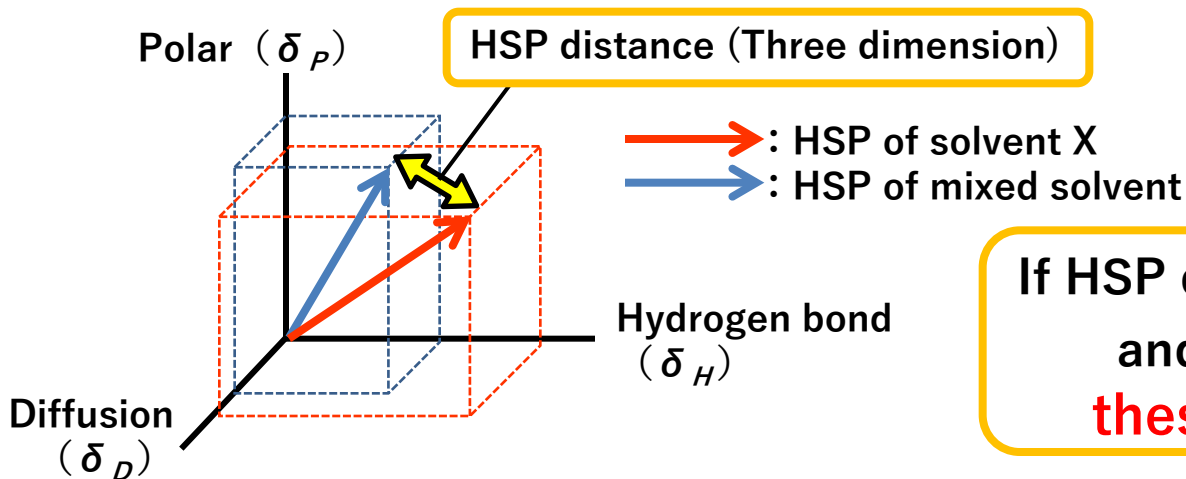
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HSP is method to separate Hildebrand solubility parameter into  $\delta_D$ :Dispersion,  $\delta_P$ :Polar,  $\delta_H$ :hydrogen bonding.

➤ Hildebrand  $\delta = (\Delta E^V/V)^{1/2}$

$E^V$  : Cohesive energy  
 $V$  : Molar volume

➤ Hansen  $\delta = (\Delta E_D^V/V)^{1/2} + (\Delta E_P^V/V)^{1/2} + (\Delta E_H^V/V)^{1/2}$   
 $= (\delta_D + \delta_P + \delta_H)^{1/2}$



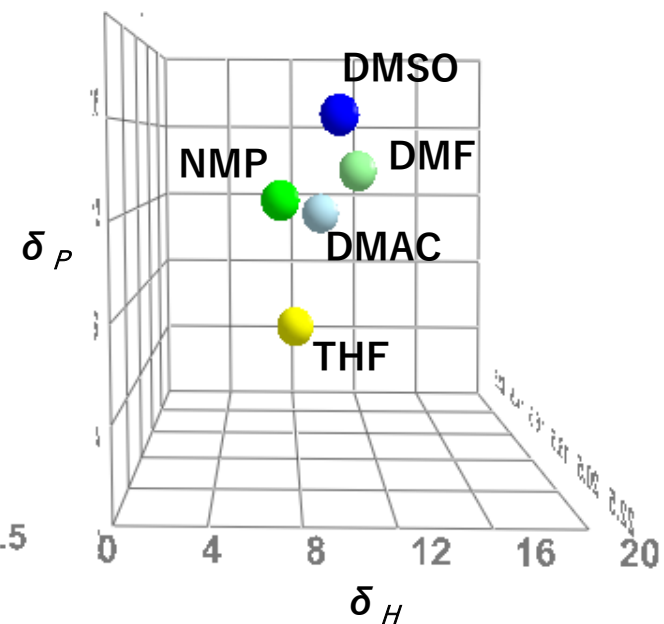
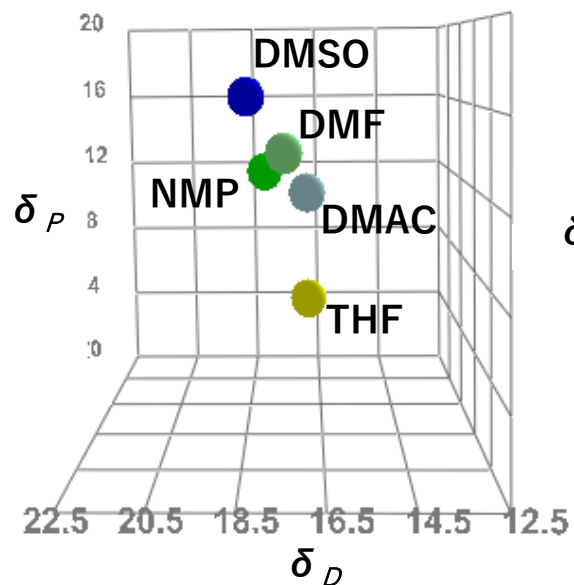
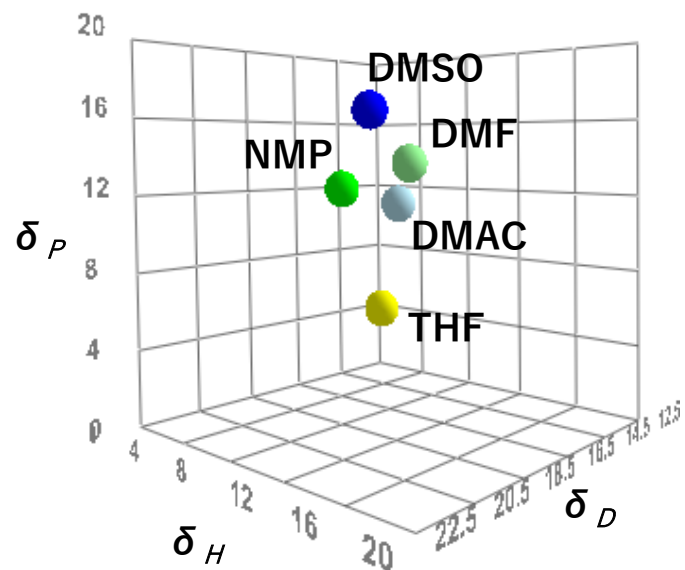
If HSP distance between solvent X and mixed solvent is near, **these solubility is similar.**

Reference : The TRC News No.120 (Feb. 2015)

# HSP of each solvents

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Solvent	$\delta_D$	$\delta_P$	$\delta_H$	HSP
DMSO	18.4	16.4	10.2	26.7
THF	16.8	5.7	8.0	19.5
NMP	18.0	12.3	7.2	23.0
DMF	17.4	13.7	11.3	24.9
DMAC	16.8	11.5	9.4	22.4



# Result of the Survey to alter NMP, DMF, DMAC

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## Calculation result by HSP software

Target solvent	Solvent 1 Vol.%	Solvent 2 Vol.%	Solvent 3 Vol.%	$\delta_D$	$\delta_P$	$\delta_H$	HSP Distance
NMP	<b>DMSO</b> 46	Solvent A 54	—	18.1	12.1	7.4	0.4
NMP	<b>DMSO</b> 50	Solvent B 36	Solvent C 14	18.0	12.3	7.2	0
NMP	<b>DMSO</b> 41	<b>THF</b> 11	Solvent D 48	17.7	12.2	7.6	0.7
DMF	<b>DMSO</b> 74	Solvent G 26	—	17.6	13.5	11.4	0.4
DMF	<b>DMSO</b> 62	Solvent H 27	Solvent I 11	17.4	13.7	11.3	0
DMF	<b>DMSO</b> 65	<b>THF</b> 21	Solvent J 14	17.5	13.6	11.4	0.3
DMAC	<b>DMSO</b> 40	Solvent K 60	—	16.8	11.5	10.6	0.4
DMAC	<b>THF</b> 49	Solvent L 40	Solvent M 11	17.0	11.3	10.3	0.5

A mixed solvents having near HSP to NMP, DMF, DMAC can be prepared by mixing DMSO and/or THF and other solvents.

# **TORAY**

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