



## Survey in Data of Solvents

Dr. Nagham Mahmood Aljamali

Review Article

Assist. Professor in Organic Chemistry ,  
Chemistry Department .,College of Education .,Kufa University .,IRAQ

### CORRESPONDING AUTHOR ADDRESS

Dr. Nagham Mahmood Aljamali

Assist. Professor in Organic Chemistry , Chemistry Department .,College of Education .,Kufa University .,IRAQ.

E-mail :dr.nagham\_mj@yahoo.com

#### Abstract:

In this paper ., types of organic solvents , degree of polarity , type of polarity , solvation of compounds in various solvents ., melting points of some compounds , boiling points of solvents, preparation of solvents , choosing of solvent for reactions .

Keyword: liquid , choosing , proton.

#### Introduction:

Solvents can cause considerable confusion in reactions, because they're listed along with the reagents of a reaction but often don't actually participate in the reaction itself. A solvent is a **liquid** that serves as the medium for a reaction. It can serve two major purposes:

1. (Non-participatory) **to dissolve the reactants**. Remember "like dissolves like" ? Polar solvents are best for dissolving polar reactants (such as ions); nonpolar solvents are best for dissolving nonpolar reactants (such as hydrocarbons).
2. Participatory: as a source of **acid** (proton), **base** (removing protons), or as a **nucleophile**(donating a lone pair of electrons). The only class of solvents for which this is something you generally need to worry about are polar protic solvents (see below).

OK. So what does "polar" and "non-polar" mean?

**Polar solvents** have large dipole moments (aka "partial charges"); they contain bonds between atoms with very different electronegativities, such as oxygen and hydrogen.

**Non polar solvents** contain bonds between atoms with similar electronegativities, such as carbon and hydrogen (think hydrocarbons, such as gasoline). Bonds between atoms with

similar electronegativities will lack partial charges; it's this absence of charge which makes these molecules "non-polar".

There are two common ways of measuring this polarity. One is through measuring a constant called "dielectric constant" or permittivity. The greater the dielectric constant, the greater the polarity (water = high, gasoline = low). A second comes from directly measuring the dipole moment.

There's a final distinction to be made and this causes confusion. Some solvents are called "protic" and some are called "aprotic". What makes a solvent a "protic" solvent, anyway?

- **Protic solvents** have O-H or N-H bonds. Why is this important? Because protic solvents can participate in hydrogen bonding, which is a powerful intermolecular force. Additionally, these O-H or N-H bonds can serve as a source of protons (H<sup>+</sup>).
- **Aprotic solvents** may have hydrogens on them somewhere, but they lack O-H or N-H bonds, and therefore **cannot hydrogen bond** with themselves.





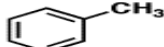
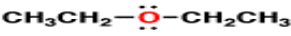

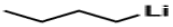

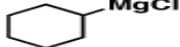
For the average first semester student, these distinctions come up the most in substitution reactions, where hydrogen bonding solvents tend to decrease the reactivity of nucleophiles; polar aprotic solvents, on the other hand, do not.

There are 3 types of solvents commonly encountered: nonpolar, polar aprotic, and polar protic. (There ain't such a thing as a non-polar protic solvent).

OK, enough yammering. Here are some (hopefully useful) tables.

#### **Nonpolar solvents:**

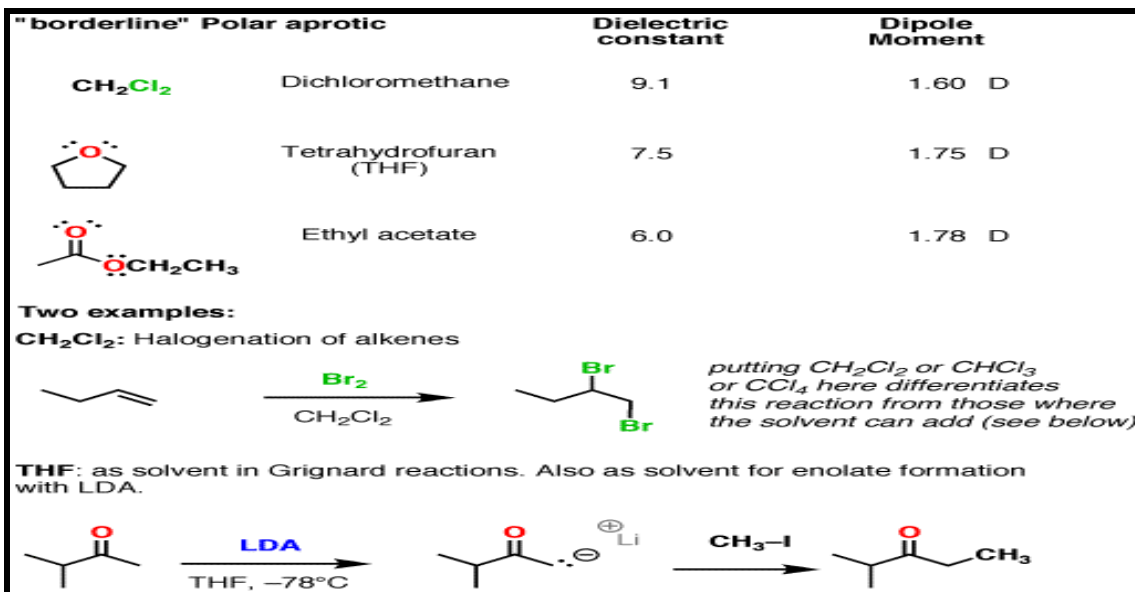
These solvents have low dielectric constants (<5) and are not good solvents for charged species such as anions. However diethyl ether (Et<sub>2</sub>O) is a common solvent for Grignard reactions; its lone pairs are Lewis basic and can help to solvate the Mg cation.

Nonpolar solvents		Dielectric constant	Dipole Moment
	Pentane	1.8	0.00 D
	Hexane	1.9	0.00 D
	Cyclohexane	2.0	0.00 D
	Benzene	2.4	0.00 D
	Toluene	2.3	0.36 D
<b>CHCl<sub>3</sub></b>	Chloroform	4.8	1.04 D
	Diethyl ether (Et <sub>2</sub> O)	4.3	1.15 D
<b>Two specific applications:</b>			
<b>Pentane:</b> Formation of organolithium reagents			
	$\xrightarrow[\text{pentane}]{\text{Li (2 equiv)}}$		+ LiBr
<b>Diethyl Ether:</b> Formation of Grignard reagents			
	$\xrightarrow[\text{Et}_2\text{O}]{\text{Mg}}$		

### Polar aprotic solvents

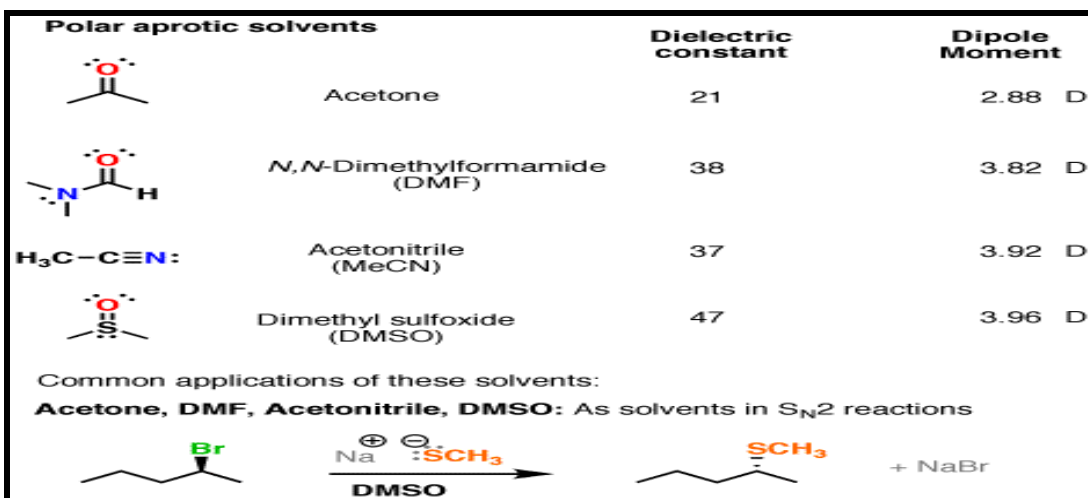
These solvents have moderately higher dielectric constants than the nonpolar solvents (between 5 and 20). Since they have intermediate polarity they are good “general purpose” solvents for a wide range of reactions. They are “aprotic” because they lack O-H or N-H bonds. For our purposes they don’t participate in reactions: they serve only as the medium.





### Polar aprotic solvents

These solvents all have large dielectric constants (>20) and large dipole moments, but they do not participate in hydrogen bonding (no O-H or N-H bonds). Their high polarity allows them to dissolve charged species such as various anions used as nucleophiles (e.g. CN<sup>-</sup>, HO<sup>-</sup>, etc.). The lack of hydrogen bonding in the solvent means that these nucleophiles are relatively "free" in solution, making them more reactive. For our purposes these solvents do not participate in the reaction.



### Polar protic solvents

Polar protic solvents tend to have high dielectric constants and high dipole moments. Furthermore, since they possess O-H or N-H bonds, they can also participate in hydrogen bonding. These solvents can also serve as acids (sources of protons) and weak nucleophiles (forming bonds with strong electrophiles).

They are most commonly used as the solvent for their conjugate bases. (e.g. H<sub>2</sub>O is used as the solvent for HO(-); EtOH is used as the solvent for EtO(-).)

Polar Protic Solvents		Dielectric constant	Dipole Moment
$\text{:NH}_3$	<i>Ammonia</i>	~25	1.4 D
$\text{H}-\ddot{\text{O}}-\text{C}(\text{CH}_3)_2-\text{CH}_3$	<i>t-Butanol</i>	12	1.7 D
$\text{H}-\ddot{\text{O}}-\text{CH}_2\text{CH}_2\text{CH}_3$	<i>n-Propanol</i>	20	1.68 D
$\text{H}-\ddot{\text{O}}-\text{CH}_2\text{CH}_3$	<i>Ethanol</i>	25	1.69 D
$\text{H}-\ddot{\text{O}}-\text{CH}_3$	<i>Methanol</i>	33	1.70 D
$\text{H}-\ddot{\text{O}}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3$	<i>Acetic acid</i>	6.2	1.74 D
$\text{H}-\ddot{\text{O}}-\text{H}$	<i>Water</i>	80	1.85 D

**Common uses:**  
**All:** As the solvent for their conjugate bases  
 e.g.  $\text{NH}_2^- / \text{NH}_3$      $\text{EtO}^- / \text{EtOH}$      $\text{HO}^- / \text{H}_2\text{O}$      $\text{t-BuO}^- / \text{t-BuOH}$   
**All:** As weak nucleophiles, in the presence of strong electrophiles (such as acid)

**Examples:**

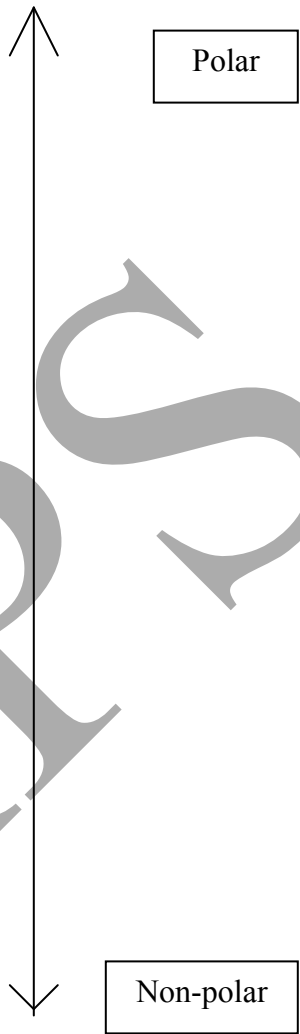
$\text{R}-\text{CH}=\text{CH}_2 \xrightarrow[\text{CH}_3\text{OH}]{\text{H}^+} \text{R}-\text{CH}(\text{OH})-\text{CH}_3$

$\text{R}-\text{CH}=\text{CH}_2 \xrightarrow[\text{H}_2\text{O}]{\text{Br}_2} \text{R}-\text{CH}(\text{OH})-\text{CH}_2\text{Br}$

These types of solvents are by far the most likely to participate in reactions. There are many examples (too many to list) where a polar protic solvent such as water, methanol, or ethanol can serve as the nucleophile in a reaction, often when a strong electrophile (such as an acid) is present. So if you see this type of solvent

Polarity of Solvents

- Water
- Acetic Acid
- Ethyleneglycol
- Methanol
- Ethanol
- Isopropanol
- Pyridine
- Acetonitrile
- Nitromethane
- Diehylamine
- Aniline
- Dimethylsulfoxide
- Ethylacetate
- Dioxane
- Acetone
- Dichloroethane
- Tetrahydrofuran
- Dicholoromethane
- Chloroform
- Diethylether
- Benzene
- Toluene
- Xylene
- Carbontetrachloride
- Cyclohexane
- Petroleum ether
- Hexane
- Pentane



Polarity Index	Solvent	Polarity Index	Solvent	Solubility in Water (%)
6.2	<input type="checkbox"/> Acetic Acid	0	Heptane	0.0003
5.1	<input type="checkbox"/> Acetone	0	Hexane	0.001
5.8	<input type="checkbox"/> Acetonitrile	0	Pentane	0.004
2.7	<input type="checkbox"/> Benzene	0.2	Cyclohexane	0.01
4	<input type="checkbox"/> n-Butanol	1	Trichloroethylene	0.11
3.9	<input type="checkbox"/> Butyl Acetate	1.6	Carbon Tetrachloride	0.08
1.6	<input type="checkbox"/> Carbon Tetrachloride	2.2	Di-Iso-Propyl Ether	0
4.1	<input type="checkbox"/> Chloroform	2.4	Toluene	0.051
0.2	<input type="checkbox"/> Cyclohexane	2.5	Methyl-t-Butyl Ether	4.8
3.5	<input type="checkbox"/> 1,2-Dichloroethane	2.5	Xylene	0.018
3.1	<input type="checkbox"/> Dichloromethane	2.7	Benzene	0.18
6.4	<input type="checkbox"/> Dimethylformamide	2.8	DiEthyl Ether	6.89
7.2	<input type="checkbox"/> Dimethyl Sulfoxide	3.1	Dichloromethane	1.6
4.8	<input type="checkbox"/> Dioxane	3.5	1,2-Dichloroethane	0.81
5.2	<input type="checkbox"/> Ethanol	3.9	Butyl Acetate	7.81
4.4	<input type="checkbox"/> Ethyl Acetate	3.9	Iso-Propanol	100
2.8	<input type="checkbox"/> DiEthyl Ether	4	n-Butanol	0.43
0	<input type="checkbox"/> Heptane	4	Tetrahydrofuran	100
0	<input type="checkbox"/> Hexane	4	n-Propanol	100
5.1	<input type="checkbox"/> Methanol	4.1	Chloroform	0.815
2.5	<input type="checkbox"/> Methyl-t-Butyl Ether	4.4	Ethyl Acetate	8.7
4.7	<input type="checkbox"/> 2-Butanone	4.7	2-Butanone	24
0	<input type="checkbox"/> Pentane	4.8	Dioxane	100

4	<input type="checkbox"/>	n-Propanol	5.1	Acetone	100
3.9	<input type="checkbox"/>	Iso-Propanol	5.1	Methanol	100
2.2	<input type="checkbox"/>	Di-Iso-Propyl Ether	5.2	Ethanol	100
4	<input type="checkbox"/>	Tetrahydrofuran	5.8	Acetonitrile	100
2.4	<input type="checkbox"/>	Toluene	6.2	Acetic Acid	100
1	<input type="checkbox"/>	Trichloroethylene	6.4	Dimethylformamide	100
9	<input type="checkbox"/>	Water	7.2	Dimethyl Sulfoxide	100
2.5	<input type="checkbox"/>	Xylene	9	Water	100

### Properties of Organic Solvents

The values in the table below except as noted have been extracted from online and hardbound compilations. Values for relative polarity, eluant strength, threshold limits and vapor pressure have been extracted from: Christian Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Publishers, 3rd ed., 2003.

Table 1 arranged alphabetically, Table 2 arranged according to increasing polarity

Solvent	formula	boilingpoint(°C)	meltingpoint(°C)	density (g/mL)	solubilityin H <sub>2</sub> O <sup>1</sup> (g/100g)	relative polarity <sup>2</sup>
acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	118	16.6	1.049	M	0.648
acetone	C <sub>3</sub> H <sub>6</sub> O	56.2	-94.3	0.786	M	0.355
acetonitrile	C <sub>2</sub> H <sub>3</sub> N	81.6	-46	0.786	M	0.460
acetyl acetone	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	140.4	-23	0.975	16	0.571
2-aminoethanol	C <sub>2</sub> H <sub>7</sub> NO	170.9	10.5	1.018	M	0.651
aniline	C <sub>6</sub> H <sub>7</sub> N	184.4	-6.0	1.022	3.4	0.420
anisole	C <sub>7</sub> H <sub>8</sub> O	153.7	-37.5	0.996	0.10	0.198
benzene	C <sub>6</sub> H <sub>6</sub>	80.1	5.5	0.879	0.18	0.111
benzonitrile	C <sub>7</sub> H <sub>5</sub> N	205	-13	0.996	0.2	0.333
benzyl alcohol	C <sub>7</sub> H <sub>8</sub> O	205.4	-15.3	1.042	3.5	0.608

1-butanol	C <sub>4</sub> H <sub>10</sub> O	117.6	-89.5	0.81	7.7	0.586
2-butanol	C <sub>4</sub> H <sub>10</sub> O	99.5	-114.7	0.808	18.1	0.506
<i>i</i> -butanol	C <sub>4</sub> H <sub>10</sub> O	107.9	-108.2	0.803	8.5	0.552
2-butanone	C <sub>4</sub> H <sub>8</sub> O	79.6	-86.3	0.805	25.6	0.327
<i>t</i> -butyl alcohol	C <sub>4</sub> H <sub>10</sub> O	82.2	25.5	0.786	M	0.389
carbon disulfide	CS <sub>2</sub>	46.3	-111.6	1.263	0.2	0.065
carbon tetrachloride	CCl <sub>4</sub>	76.7	-22.4	1.594	0.08	0.052
chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	132	-45.6	1.106	0.05	0.188
chloroform	CHCl <sub>3</sub>	61.2	-63.5	1.498	0.8	0.259
cyclohexane	C <sub>6</sub> H <sub>12</sub>	80.7	6.6	0.779	0.005	0.006
cyclohexanol	C <sub>6</sub> H <sub>12</sub> O	161.1	25.2	0.962	4.2	0.509
cyclohexanone	C <sub>6</sub> H <sub>10</sub> O	155.6	-16.4	0.948	2.3	0.281
di- <i>n</i> -butylphthalate	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	340	-35	1.049	0.0011	0.272
1,1-dichloroethane	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	57.3	-97.0	1.176	0.5	0.269
diethylene glycol	C <sub>4</sub> H <sub>10</sub> O <sub>3</sub>	245	-10	1.118	M	0.713
diglyme	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>	162	-64	0.945	M	0.244
dimethoxyethane (glyme)	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	85	-58	0.868	M	0.231
<i>N,N</i> -dimethylaniline	C <sub>8</sub> H <sub>11</sub> N	194.2	2.4	0.956	0.14	0.179
dimethylformamide (DMF)	C <sub>3</sub> H <sub>7</sub> NO	153	-61	0.944	M	0.386
dimethylphthalate	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	283.8	1	1.190	0.43	0.309
dimethylsulfoxide (DMSO)	C <sub>2</sub> H <sub>6</sub> OS	189	18.4	1.092	M	0.444
dioxane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	101.1	11.8	1.033	M	0.164

ethanol	C <sub>2</sub> H <sub>6</sub> O	78.5	-114.1	0.789	M	0.654
ether	C <sub>4</sub> H <sub>10</sub> O	34.6	-116.3	0.713	7.5	0.117
ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	77	-83.6	0.894	8.7	0.228
ethyl acetoacetate	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	180.4	-80	1.028	2.9	0.577
ethyl benzoate	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	213	-34.6	1.047	0.07	0.228
ethylene glycol	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	197	-13	1.115	M	0.790
glycerin	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>	290	17.8	1.261	M	0.812
heptane	C <sub>7</sub> H <sub>16</sub>	98	-90.6	0.684	0.0003	0.012
1-heptanol	C <sub>7</sub> H <sub>16</sub> O	176.4	-35	0.819	0.17	0.549
hexane	C <sub>6</sub> H <sub>14</sub>	69	-95	0.655	0.0014	0.009
1-hexanol	C <sub>6</sub> H <sub>14</sub> O	158	-46.7	0.814	0.59	0.559
methanol	CH <sub>4</sub> O	64.6	-98	0.791	M	0.762
methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	56.9	-98.1	0.933	24.4	0.253
methyl <i>t</i> -butyl ether (MTBE)	C <sub>5</sub> H <sub>12</sub> O	55.2	-109	0.741	4.8	0.124
methylene chloride	CH <sub>2</sub> Cl <sub>2</sub>	39.8	-96.7	1.326	1.32	0.309
1-octanol	C <sub>8</sub> H <sub>18</sub> O	194.4	-15	0.827	0.096	0.537
pentane	C <sub>5</sub> H <sub>12</sub>	36.1	-129.7	0.626	0.004	0.009
1-pentanol	C <sub>5</sub> H <sub>12</sub> O	138.0	-78.2	0.814	2.2	0.568
2-pentanol	C <sub>5</sub> H <sub>12</sub> O	119.0	-50	0.810	4.5	0.488
3-pentanol	C <sub>5</sub> H <sub>12</sub> O	115.3	-8	0.821	5.1	0.463
2-pentanone	C <sub>5</sub> H <sub>10</sub> O	102.3	-76.9	0.809	4.3	0.321
3-pentanone	C <sub>5</sub> H <sub>12</sub> O	101.7	-39.8	0.814	3.4	0.265
1-propanol	C <sub>3</sub> H <sub>8</sub> O	97	-126	0.803	M	0.617
2-propanol	C <sub>3</sub> H <sub>8</sub> O	82.4	-88.5	0.785	M	0.546
pyridine	C <sub>5</sub> H <sub>5</sub> N	115.5	-42	0.982	M	0.302
tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O	66	-108.4	0.886	30	0.207

THF)						
toluene	C <sub>7</sub> H <sub>8</sub>	110.6	-93	0.867	0.05	0.099
water	H <sub>2</sub> O	100.00	0.00	0.998	M	1.000
water, heavy	D <sub>2</sub> O	101.3	4	1.107	M	0.991
<i>p</i> -xylene	C <sub>8</sub> H <sub>10</sub>	138.3	13.3	0.861	0.02	0.074

- 1 M = miscible.
- 2 The values for relative polarity are normalized from measurements of solvent shifts of absorption spectra and were extracted from Christian Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Publishers, 3rd ed., 2003.
- 3 Snyder's empirical eluant strength parameter for alumina. Extracted from Reichardt, page 495.
- 4 Threshold limits for exposure. Extracted from Reichardt, pages 501-502.

TABLE 2

Solvent	formula	Boiling point(°C)	Melting point(°C)	density (g/mL)	Solubility in H <sub>2</sub> O <sup>1</sup> (g/100g)	relative polarity <sup>2</sup>	threshold limits <sup>4</sup> (ppm)
cyclohexane	C <sub>6</sub> H <sub>12</sub>	80.7	6.6	0.779	0.005	0.006	100
pentane	C <sub>5</sub> H <sub>12</sub>	36.1	-129.7	0.626	0.0039	0.009	600
hexane	C <sub>6</sub> H <sub>14</sub>	69	-95	0.655	0.0014	0.009	50
heptane	C <sub>7</sub> H <sub>16</sub>	98	-90.6	0.684	0.0003	0.012	400
carbon tetrachloride	CCl <sub>4</sub>	76.7	-22.4	1.594	0.08	0.052	5
carbon disulfide	CS <sub>2</sub>	46.3	-111.6	1.263	0.2	0.065	10
<i>p</i> -xylene	C <sub>8</sub> H <sub>10</sub>	138.3	13.3	0.861	0.02	0.074	100
toluene	C <sub>7</sub> H <sub>8</sub>	110.6	-93	0.867	0.05	0.099	50
benzene	C <sub>6</sub> H <sub>6</sub>	80.1	5.5	0.879	0.18	0.111	0.5
ether	C <sub>4</sub> H <sub>10</sub> O	34.6	-116.3	0.713	7.5	0.117	400
methyl <i>t</i> -butyl ether (MTBE)	C <sub>5</sub> H <sub>12</sub> O	55.2	-109	0.741	4.8	0.124	

diethylamine	C <sub>4</sub> H <sub>11</sub> N	56.3	-48	0.706	M	<b>0.145</b>	5
dioxane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	101.1	11.8	1.033	M	<b>0.164</b>	20
N,N-dimethylaniline	C <sub>8</sub> H <sub>11</sub> N	194.2	2.4	0.956	0.14	<b>0.179</b>	
chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	132	-45.6	1.106	0.05	<b>0.188</b>	10
anisole	C <sub>7</sub> H <sub>8</sub> O	153.7	-37.5	0.996	0.10	<b>0.198</b>	
tetrahydrofuran (THF)	C <sub>4</sub> H <sub>8</sub> O	66	-108.4	0.886	30	<b>0.207</b>	200
ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	77	-83.6	0.894	8.7	<b>0.228</b>	400
ethyl benzoate	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	213	-34.6	1.047	0.07	<b>0.228</b>	
dimethoxyethane (glyme)	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	85	-58	0.868	M	<b>0.231</b>	
diglyme	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>	162	-64	0.945	M	<b>0.244</b>	
methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	56.9	-98.1	0.933	24.4	<b>0.253</b>	200
chloroform	CHCl <sub>3</sub>	61.2	-63.5	1.498	0.8	<b>0.259</b>	10
3-pentanone	C <sub>5</sub> H <sub>12</sub> O	101.7	-39.8	0.814	3.4	<b>0.265</b>	200
1,1-dichloroethane	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	57.3	-97.0	1.176	0.5	<b>0.269</b>	100
di-n-butyl phthalate	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	340	-35	1.049	0.0011	<b>0.272</b>	
cyclohexanone	C <sub>6</sub> H <sub>10</sub> O	155.6	-16.4	0.948	2.3	<b>0.281</b>	25
pyridine	C <sub>5</sub> H <sub>5</sub> N	115.5	-42	0.982	M	<b>0.302</b>	5
dimethylphthalate	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	283.8	1	1.190	0.43	<b>0.309</b>	
methylene chloride	CH <sub>2</sub> Cl <sub>2</sub>	39.8	-96.7	1.326	1.32	<b>0.309</b>	50
2-pentanone	C <sub>5</sub> H <sub>10</sub> O	102.3	-76.9	0.809	4.3	<b>0.321</b>	
2-butanone	C <sub>4</sub> H <sub>8</sub> O	79.6	-86.3	0.805	25.6	<b>0.327</b>	200

1,2-dichloroethane	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	83.5	-35.4	1.235	0.87	<b>0.327</b>	
benzotrile	C <sub>7</sub> H <sub>5</sub> N	205	-13	0.996	0.2	<b>0.333</b>	10
acetone	C <sub>3</sub> H <sub>6</sub> O	56.2	-94.3	0.786	M	<b>0.355</b>	500
dimethylformamide (DMF)	C <sub>3</sub> H <sub>7</sub> N O	153	-61	0.944	M	<b>0.386</b>	10
<i>t</i> -butyl alcohol	C <sub>4</sub> H <sub>10</sub> O	82.2	25.5	0.786	M	<b>0.389</b>	100
aniline	C <sub>6</sub> H <sub>7</sub> N	184.4	-6.0	1.022	3.4	<b>0.420</b>	2
dimethylsulfoxide (DMSO)	C <sub>2</sub> H <sub>6</sub> O S	189	18.4	1.092	M	<b>0.444</b>	
acetonitrile	C <sub>2</sub> H <sub>3</sub> N	81.6	-46	0.786	M	<b>0.460</b>	20
3-pentanol	C <sub>5</sub> H <sub>12</sub> O	115.3	-8	0.821	5.1	<b>0.463</b>	
2-pentanol	C <sub>5</sub> H <sub>12</sub> O	119.0	-50	0.810	4.5	<b>0.488</b>	
2-butanol	C <sub>4</sub> H <sub>10</sub> O	99.5	-114.7	0.808	18.1	<b>0.506</b>	100
cyclohexanol	C <sub>6</sub> H <sub>12</sub> O	161.1	25.2	0.962	4.2	<b>0.509</b>	50
1-octanol	C <sub>8</sub> H <sub>18</sub> O	194.4	-15	0.827	0.096	<b>0.537</b>	
2-propanol	C <sub>3</sub> H <sub>8</sub> O	82.4	-88.5	0.785	M	<b>0.546</b>	400
1-heptanol	C <sub>7</sub> H <sub>16</sub> O	176.4	-35	0.819	0.17	<b>0.549</b>	
<i>i</i> -butanol	C <sub>4</sub> H <sub>10</sub> O	107.9	-108.2	0.803	8.5	<b>0.552</b>	
1-hexanol	C <sub>6</sub> H <sub>14</sub> O	158	-46.7	0.814	0.59	<b>0.559</b>	
1-pentanol	C <sub>5</sub> H <sub>12</sub> O	138.0	-78.2	0.814	2.2	<b>0.568</b>	
acetyl acetone	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	140.4	-23	0.975	16	<b>0.571</b>	
ethyl acetoacetate	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	180.4	-80	1.028	2.9	<b>0.577</b>	
1-butanol	C <sub>4</sub> H <sub>10</sub> O	117.6	-89.5	0.81	7.7	<b>0.586</b>	20
benzyl alcohol	C <sub>7</sub> H <sub>8</sub> O	205.4	-15.3	1.042	3.5	<b>0.608</b>	
1-propanol	C <sub>3</sub> H <sub>8</sub> O	97	-126	0.803	M	<b>0.617</b>	
acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	118	16.6	1.049	M	<b>0.648</b>	10

2-aminoethanol	C <sub>2</sub> H <sub>7</sub> N O	170.9	10.5	1.018	M	0.651	3
ethanol	C <sub>2</sub> H <sub>6</sub> O	78.5	-114.1	0.789	M	0.654	1000
diethylene glycol	C <sub>4</sub> H <sub>10</sub> O 3	245	-10	1.118	M	0.713	
methanol	CH <sub>4</sub> O	64.6	-98	0.791	M	0.762	200
ethylene glycol	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	197	-13	1.115	M	0.790	
glycerin	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>	290	17.8	1.261	M	0.812	
water, heavy	D <sub>2</sub> O	101.3	4	1.107	M	0.991	
water	H <sub>2</sub> O	100.00	0.00	0.998	M	1.000	

NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities *Organometallics*, 2010, 29 (9), pp 2176–2179

Table 1. <sup>1</sup>H NMR Data<sup>a</sup>

	proton	mult	THF- <i>d</i> <sub>8</sub>	CDCl <sub>3</sub>	C <sub>6</sub> D <sub>6</sub>	(CD <sub>3</sub> ) <sub>2</sub> CO	(CD <sub>3</sub> ) <sub>2</sub> SO	TFE- <i>d</i> <sub>3</sub>	CD <sub>3</sub> OD
solvent residual signals			1.72	7.26	7.16	2.05	2.50	5.02	3.31
			3.58					3.88	
water	OH	s	2.46	1.56	0.40	2.84 <sup>b</sup>	3.33 <sup>b</sup>	3.66	4.87
acetic acid	CH <sub>3</sub>	s	1.89	2.10	1.52	1.96	1.91	2.06	1.99
acetone	CH <sub>3</sub>	s	2.05	2.17	1.55	2.09	2.09	2.19	2.15
acetonitrile	CH <sub>3</sub>	s	1.95	2.10	0.58	2.05	2.07	1.95	2.03
benzene	CH	s	7.31	7.36	7.15	7.36	7.37	7.36	7.33
<i>tert</i> -butyl alcohol	CH <sub>3</sub>	s	1.15	1.28	1.05	1.18	1.11	1.28	1.40
	OH	s <sup>c</sup>	3.16		0.63		4.19	2.20	
chloroform	CH	s	7.89	7.26	6.15	8.02	8.32	7.33	7.90
18-crown-6	CH <sub>2</sub>	s	3.57	3.67	3.39	3.59	3.51	3.64	3.64
cyclohexane	CH <sub>2</sub>	s	1.44	1.43	1.40	1.43	1.40	1.47	1.45

1,2-dichloroethane	CH <sub>2</sub>	s	3.77	3.73	2.90	3.87	3.90	3.71	3.78
dichloromethane	CH <sub>2</sub>	s	5.51	5.30	4.27	5.63	5.76	5.24	5.49
diethyl ether	CH <sub>3</sub>	t, 7	1.12	1.21	1.11	1.11	1.09	1.20	1.18
	CH <sub>2</sub>	q, 7	3.38	3.48	3.26	3.41	3.38	3.58	3.49
diglyme	CH <sub>2</sub>	m	3.43	3.65	3.46	3.56	3.51	3.67	3.61
	CH <sub>2</sub>	m	3.53	3.57	3.34	3.47	3.38	3.62	3.58
	OCH <sub>3</sub>	s	3.28	3.39	3.11	3.28	3.24	3.41	3.35
dimethylformamide	CH	s	7.91	8.02	7.63	7.96	7.95	7.86	7.97
	CH <sub>3</sub>	s	2.88	2.96	2.36	2.94	2.89	2.98	2.99
	CH <sub>3</sub>	s	2.76	2.88	1.86	2.78	2.73	2.88	2.86
1,4-dioxane	CH <sub>2</sub>	s	3.56	3.71	3.35	3.59	3.57	3.76	3.66
DME	CH <sub>3</sub>	s	3.28	3.40	3.12	3.28	3.24	3.40	3.35
	CH <sub>2</sub>	s	3.43	3.55	3.33	3.46	3.43	3.61	3.52
ethane	CH <sub>3</sub>	s	0.85	0.87	0.80	0.83	0.82	0.85	0.85
ethanol	CH <sub>3</sub>	t, 7	1.10	1.25	0.96	1.12	1.06	1.22	1.19
	CH <sub>2</sub>	q, 7 <sup>d</sup>	3.51	3.72	3.34	3.57	3.44	3.71	3.60
	OH	s <sup>c,d</sup>	3.30	1.32	0.50	3.39	4.63		
ethyl acetate	CH <sub>3</sub> CO	s	1.94	2.05	1.65	1.97	1.99	2.03	2.01
	CH <sub>2</sub> CH <sub>3</sub>	q, 7	4.04	4.12	3.89	4.05	4.03	4.14	4.09
	CH <sub>2</sub> CH <sub>3</sub>	t, 7	1.19	1.26	0.92	1.20	1.17	1.26	1.24
ethylene	CH <sub>2</sub>	s	5.36	5.40	5.25	5.38	5.41	5.40	5.39
ethylene glycol	CH <sub>2</sub>	s <sup>e</sup>	3.48	3.76	3.41	3.28	3.34	3.72	3.59
H grease <sup>f</sup>	CH <sub>3</sub>	m	0.85-0.91	0.84-0.87	0.90-0.98	0.90	0.82-0.88	0.88-0.94	0.86-0.93
	CH <sub>2</sub>	br s	1.29	1.25	1.32	1.29	1.24	1.33	1.29
hexamethylbenzene	CH <sub>3</sub>	s	2.18	2.24	2.13	2.17	2.14	2.24	2.19
n-hexane	CH <sub>3</sub>	t, 7	0.89	0.88	0.89	0.88	0.86	0.91	0.90
	CH <sub>2</sub>	m	1.29	1.26	1.24	1.28	1.25	1.31	1.29
HMDSO	CH <sub>3</sub>	s	0.07	0.07	0.12	0.07	0.06	0.08	0.07
HMPA	CH <sub>3</sub>	d,9.5	2.58	2.65	2.40	2.59	2.53	2.63	2.64
hydrogen	H <sub>2</sub>	s	4.55	4.62	4.47	4.54	4.61	4.53	4.56
imidazole	CH(2)	s	7.48	7.67	7.33	7.62	7.63	7.61	7.67
	CH(4,5)	s	6.94	7.10	6.90	7.04	7.01	7.03	7.05

methane	CH <sub>4</sub>	s	0.19	0.22	0.16	0.17	0.20	0.18	0.20
methanol	CH <sub>3</sub>	s <sup>a</sup>	3.27	3.49	3.07	3.31	3.16	3.44	3.34
	OH	s <sup>c,g</sup>	3.02	1.09		3.12	4.01		
nitromethane	CH <sub>3</sub>	s	4.31	4.33	2.94	4.43	4.42	4.28	4.34
<i>n</i> -pentane	CH <sub>3</sub>	t, 7	0.89	0.88	0.87	0.88	0.86	0.90	0.90
	CH <sub>2</sub>	m	1.31	1.27	1.23	1.27	1.27	1.33	1.29
propane	CH <sub>3</sub>	t, 7.3	0.90	0.90	0.86	0.88	0.87	0.90	0.91
	CH <sub>2</sub>	sept, 7.3	1.33	1.32	1.26	1.31	1.29	1.33	1.34
2-propanol	CH <sub>3</sub>	d, 6	1.08	1.22	0.95	1.10	1.04	1.20	1.50
	CH	sept, 6	3.82	4.04	3.67	3.90	3.78	4.05	3.92
propylene	CH <sub>3</sub>	dt, 6.4, 1.5	1.69	1.73	1.55	1.68	1.68	1.70	1.70
	CH <sub>2</sub> (1)	dm, 10	4.89	4.94	4.95	4.90	4.94	4.93	4.91
	CH <sub>2</sub> (2)	dm, 17	4.99	5.03	5.01	5.00	5.03	5.03	5.01
	CH	m	5.79	5.83	5.72	5.81	5.80	5.87	5.82
pyridine	CH(2,6)	m	8.54	8.62	8.53	8.58	8.58	8.45	8.53
	CH(3,5)	m	7.25	7.29	6.66	7.35	7.39	7.40	7.44
	CH(4)	m	7.65	7.68	6.98	7.76	7.79	7.82	7.85
pyrrole	NH	br t	9.96	8.40	7.80	10.02	10.75		
	CH(2,5)	m	6.66	6.83	6.48	6.77	6.73	6.84	6.72
	CH(3,4)	m	6.02	6.26	6.37	6.07	6.01	6.24	6.08
pyrrolidine <sup>h</sup>	CH <sub>2</sub> (2,5)	m	2.75	2.87	2.54		2.67	3.11	2.80
	CH <sub>2</sub> (3,4)	m	1.59	1.68	1.33		1.55	1.93	1.72
silicone grease	CH <sub>3</sub>	s	0.11	0.07	0.29	0.13	-0.06	0.16	0.10
tetrahydrofuran	CH <sub>2</sub> (2,5)	m	3.62	3.76	3.57	3.63	3.60	3.78	3.71
	CH <sub>2</sub> (3,4)	m	1.79	1.85	1.40	1.79	1.76	1.91	1.87
toluene	CH <sub>3</sub>	s	2.31	2.36	2.11	2.32	2.30	2.33	2.32
	CH(2,4,6)	m	7.10	7.17	7.02	7.10-7.20	7.18	7.10-7.30	7.16
	CH(3,5)	m	7.19	7.25	7.13	7.10-7.20	7.25	7.10-7.30	7.16
triethylamine	CH <sub>3</sub>	t, 7	0.97	1.03	0.96	0.96	0.93	1.31	1.05
	CH <sub>2</sub>	q,7	2.46	2.53	2.40	2.45	2.43	3.12	2.58

**a**-Except for the compounds in solutions 8-10, as well as the gas samples, hexamethylbenzene, and the corrected values mentioned in the **Supporting Information**, all data for the solvents CDCl<sub>3</sub>, C<sub>6</sub>D<sub>6</sub>, (CD<sub>3</sub>)<sub>2</sub>CO, (CD<sub>3</sub>)<sub>2</sub>SO, CD<sub>3</sub>CN, CD<sub>3</sub>OD, and D<sub>2</sub>O were previously reported in ref 2.

**b**-A signal for HDO is also observed in  $(\text{CD}_3)_2\text{SO}$  (3.30 ppm) and  $(\text{CD}_3)_2\text{CO}$  (2.81 ppm), often seen as a 1:1:1 triplet ( $^2J_{\text{H,D}} = 1 \text{ Hz}$ ).

**c**-Not all OH signals were observable.

**d**-In some solvents, the coupling interaction between the  $\text{CH}_2$  and the OH protons may be observed ( $J = 5 \text{ Hz}$ ).

**e**-In  $\text{CD}_3\text{CN}$ , the OH proton was seen as a multiplet at 2.69 ppm, as well as extra coupling to the  $\text{CH}_2$  resonance.

**f**-Apiezon brand H grease.

**g**-In some solvents, a coupling interaction between the  $\text{CH}_3$  and the OH protons may be observed ( $J = 5.5 \text{ Hz}$ ).

**h**-Pyrrolidine was observed to react with  $(\text{CD}_3)_2\text{CO}$ .

### References :

- 1- Y. Ju, D. Kumar, R. S. Varma, *J. Org. Chem.*, 2006, 71, 6697-6700.
- 2- N. Iranpoor, H. Firouzabadi, B. Akhlaghinia, R. Azadi, *Synthesis*, 2004, 92-96.
- 3- Y. Liu, Y. Xu, S. H. Jung, J. Chae, *Synlett*, 2012, 2663-2666.
- 4- D. S. Bhalerao, K. G. Agamanchi, *Synlett*, 2007, 2952-2956.
- 5- J. S. Yadav, B. V. S. Reddy, U. V. S. Reddy, D. N. Chary, *Synthesis*, 2008, 1283-1287.
- 6- J. Jiao, L. X. Nguyen, D. R. Patterson, R. A. Flowers II, *Org. Lett.*, 2007, 9, 1323-1326.
- 7- J. S. Yadav, B. V. S. Reddy, M. K. Gupta, *Synthesis*, 2004, 1983-1986
- 8- S. George ., "Organic Chemistry" Mosby-Year Book . 1995 , Chp.14 , p. 589-649 (1995).
- 9- P. Sykes ; "Agide Book to Mechanism in Oaganic Chemistry" , 5<sup>th</sup> Ed ., Longman, (1974) .
- 10- R . E . Brewster , W. E. McEwen ; "Organic Chemistry" , Ch . 30<sup>ed</sup> Ed ., p.638.
- 11- Nagham M Aljamali ., *As. J. Rech.*, 2014 , 7 ,11.
- 12- Nagham M Aljamali., *Int. J. Curr.Res.Chem.Pharma.Sci.* 1(9):(2014):121–151.
- 13- Nagham M Aljamali., *Int. J. Curr.Res.Chem.Pharma.Sci.* 1(9): (2014):88- 120.