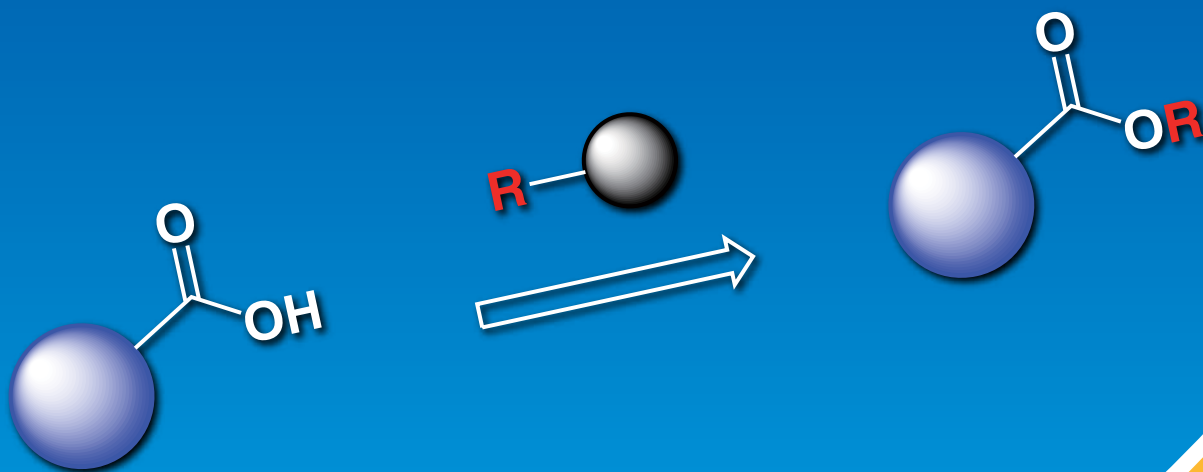


# Alkylation Reagents for Ester Synthesis



Methylation Reagents

Ethylation Reagents

Propylation & Isopropylation Reagents

Butylation & *tert*-Butylation Reagents

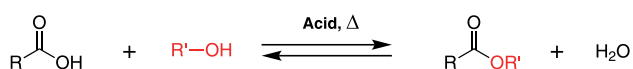
Other Alkylation Reagents



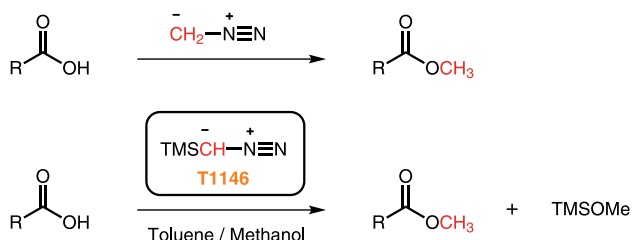
# Alkylation Reagents for Ester Synthesis

Carboxylic acid esters are basic compounds in organic chemistry, and have a wide range of uses as various chemical products such as pharmaceuticals, agrochemicals, cosmetics, flavors, and electronic materials, and their synthetic intermediates.

As for synthetic methods of ester compounds, 'Fisher esterification' is well-known since a long time ago, by which ester compounds can be synthesized using carboxylic acids and alcohols in the presence of acid catalysts.<sup>1)</sup> This reaction is reversible, and it is possible to obtain the desired esters by using excess amount of alcohols, or removing water under azeotropic condition.

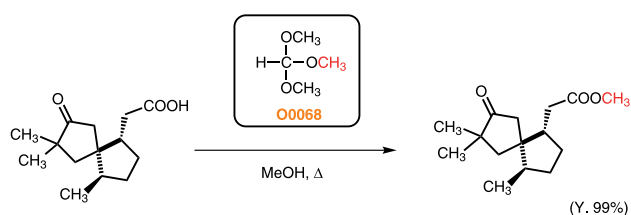


As other traditional synthetic method, the methylation reaction of carboxylic acids is also known using *in situ* generated diazomethane. This reaction proceeds fast under neutral condition. However, since there are several reports on the explosive and cancer-causing property of diazomethane, trimethylsilyldiazomethane – hexane solution (**T1146**), which is less explosive, has been used as an alternative to diazomethane in recent years.<sup>2)</sup>

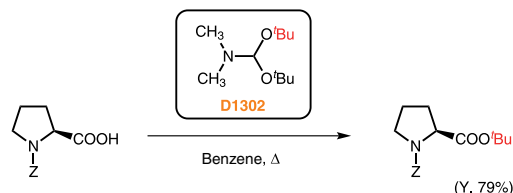


In addition to these reactions above, various kinds of synthetic methods for ester synthesis by alkylating carboxylic acids have been also reported as below.

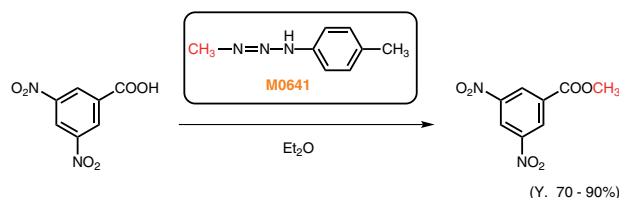
## 1. Alkylation of Carboxylic Acids using Orthoesters<sup>3)</sup>



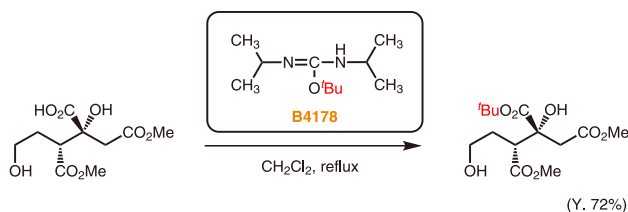
## 2. Alkylation of Carboxylic Acids using *N,N*-Dimethylformamide Dialkyl Acetals<sup>4)</sup>



## 3. Alkylation of Carboxylic Acids using Triazene Derivatives<sup>5)</sup>



## 4. Alkylation of Carboxylic Acids using *O*-Dialkylisoureas<sup>6)</sup>

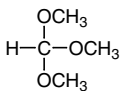
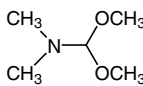
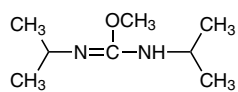
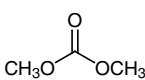
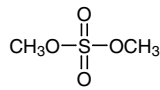
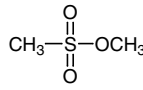
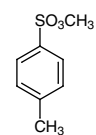
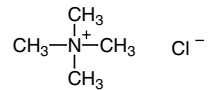
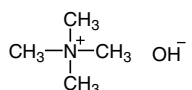
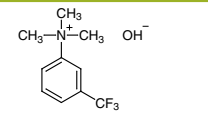
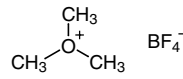
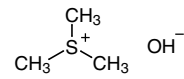
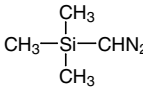
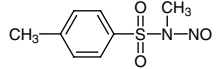
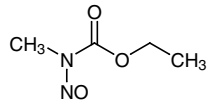
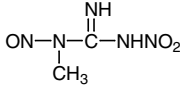
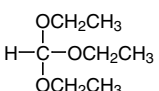
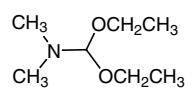
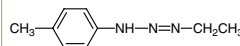


TCI offers a variety of alkylation reagents for ester synthesis other than the reagents above. All the products are listed as below.

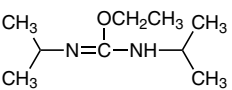
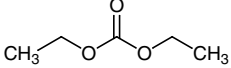
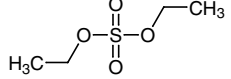
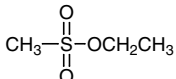
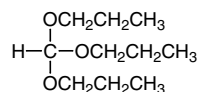
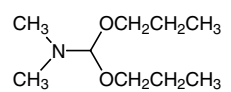
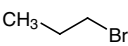
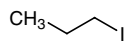
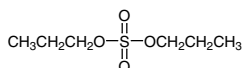
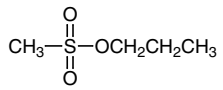
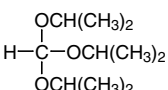
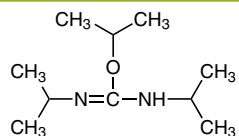
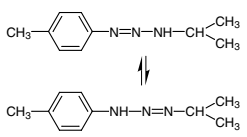
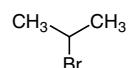
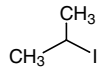
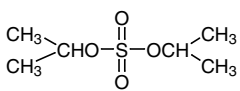
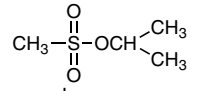
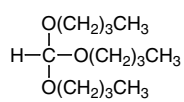
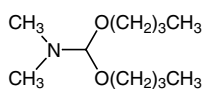
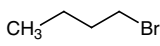
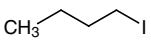
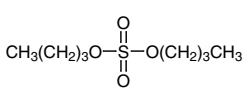
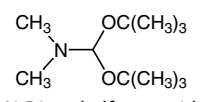
### References

- 1) E. Fischer, A. Speier, *Ber.* **1895**, 28, 3252.
- 2) T. Aoyama, T. Shioiri, *Tetrahedron Lett.* **1980**, 21, 46.
- 3) M. T. Crimmins, J. A. DeLoach, *J. Am. Chem. Soc.* **1986**, 108, 800.
- 4) U. Widmer, *Synthesis* **1983**, 135.
- 5) E. H. White, A. A. Baum, D. E. Eitel, *Org. Synth. Coll.* **1973**, 5, 797.
- 6) F. Calo, J. Richardson, A. G. M. Barrett, *J. Org. Chem.* **2008**, 73, 9692.

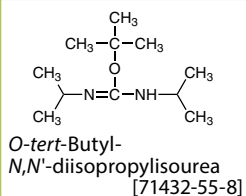
## Methylation Reagents

<b>Methylation Reagents</b>		<b>X0041</b> 25mL 100mL 500mL Hydrogen Chloride - Methanol Reagent (5-10%) [7647-01-0]	<b>X0038</b> 1set Hydrogen Chloride - Methanol Reagent (5-10%) (1mLx10) [7647-01-0]	<b>X0033</b> 1set Boron Trichloride - Methanol Reagent (5-10%) (1mLx10) [36254-91-8]
		<b>X0036</b> 1set Boron Trifluoride - Methanol Reagent (10-20%) (1mLx10) [373-57-9]	<b>O0068</b> 25mL 500mL  Trimethyl Orthoformate [149-73-5]	<b>D2071</b> 25mL  <i>N,N</i> -Dimethylformamide Dimethyl Acetal [4637-24-5]
<b>D4587</b> 5mL  <i>N,N'</i> -Diisopropyl- <i>O</i> -methylisourea [54648-79-2]	<b>B1618</b> 50g CH <sub>3</sub> Br Methyl Bromide (in cylinder without valve) [74-83-9]	<b>B3121</b> 100mL CH <sub>3</sub> Br Methyl Bromide (ca. 2mol/L in Ethyl Ether) [74-83-9]	<b>B3122</b> 100mL CH <sub>3</sub> Br Methyl Bromide (ca. 2mol/L in Tetrahydrofuran) [74-83-9]	<b>I0060</b> 10mL 100mL 300mL CH <sub>3</sub> I Methyl Iodide (stabilized with Copper chip) [74-88-4]
<b>C0053</b> 25mL 100mL 500mL  Dimethyl Carbonate [616-38-6]	<b>D0797</b> 25g 500g  Dimethyl Sulfate [77-78-1]	<b>M0369</b> 25g 100g  Methyl Methanesulfonate [66-27-3]	<b>T0269</b> 25g 500g  Methyl <i>p</i> -Toluenesulfonate [80-48-8]	<b>T0136</b> 25g 500g  Tetramethylammonium Chloride [75-57-0]
<b>T0676</b> 25mL 100mL 500mL  Tetramethylammonium Hydroxide (10% in Methanol) [75-59-2]	<b>T0961</b> 25mL  3-(Trifluoromethyl)-phenyltrimethylammonium Hydroxide (5% in Methanol) [68254-41-1]	<b>T1507</b> 5g 25g  Trimethyloxonium Tetrafluoroborate [420-37-1]	<b>T1576</b> 5mL 25mL  Trimethylsulfonium Hydroxide (0.2mol/L in Methanol) [17287-03-5]	
<b>Methylation Reagents (Diazomethane Precursors &amp; Equivalents)</b>		<b>T1146</b> 10mL 25mL 100mL  Trimethylsilyldiazomethane (ca. 10% in Hexane, ca. 0.6mol/L) [18107-18-1]	<b>T0323</b> 25g 500g  <i>N</i> -Methyl- <i>N</i> -nitroso- <i>p</i> -toluenesulfonamide [80-11-5]	<b>N0265</b> 5g 25g  <i>N</i> -Methyl- <i>N</i> -nitrosourea [615-53-2]
		<b>M0527</b> 5g 25g  1-Methyl-3-nitro-1-nitrosoguanidine (wetted with ca. 50% Water) (unit weight on dry weight basis) [70-25-7]		
<b>Ethylation Reagents</b>		<b>O0066</b> 25mL 500mL  Triethyl Orthoformate [122-51-0]	<b>D1294</b> 5mL 25mL  <i>N,N</i> -Dimethylformamide Diethyl Acetal [1188-33-6]	<b>E0292</b> 1g  1-Ethyl-3- <i>p</i> -tolyltriazene [50707-40-9]

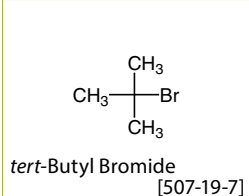
## Alkylation Reagents for Ester Synthesis

<b>E1058</b> 5mL 25mL  O-Ethyl-N,N'-diisopropylisourea [60683-30-9]	<b>B0588</b> 25g 500g $\text{CH}_3\text{CH}_2\text{Br}$ Ethyl Bromide [74-96-4]	<b>I0058</b> 25g 100g 500g $\text{CH}_3\text{CH}_2\text{I}$ Ethyl Iodide (stabilized with Copper chip) [75-03-6]	<b>C0041</b> 25g 500g  Diethyl Carbonate [105-58-8]	<b>D0525</b> 25mL 500mL  Diethyl Sulfate [64-67-5]
<b>M0607</b> 25g 100g  Ethyl Methanesulfonate [62-50-0]	<div style="background-color: #4CAF50; color: white; padding: 10px; text-align: center;"> <h3>Propylation &amp; Isopropylation Reagents</h3> </div>			
	<b>X0037</b> 1set Boron Trifluoride - Propanol Reagent (10-20%) (1mLx10) [762-48-1]	<b>O0259</b> 25mL 500mL  Tripropyl Orthoformate [621-76-1]	<b>D1301</b> 5mL 25mL  N,N-Dimethylformamide Dipropyl Acetal [6006-65-1]	
<b>B0638</b> 25g 500g  Propyl Bromide [106-94-5]	<b>I0068</b> 25g 100g 500g  Propyl Iodide (stabilized with Copper chip) [107-08-4]	<b>D1638</b> 25g 500g  Dipropyl Sulfate [598-05-0]	<b>P1844</b> 5g 25g  Propyl Methanesulfonate [1912-31-8]	<b>X0035</b> 1set Boron Trifluoride - Isopropyl Alcohol Reagent (10-20%) (1mLx10) [676-65-3]
<b>O0215</b> 25mL  Triisopropoxymethane [4447-60-3]	<b>T3123</b> 5mL 25mL  O,N,N'-Triisopropylisourea [63460-32-2]	<b>I0280</b> 1g  1-Isopropyl-3-p-tolyltriazenes [50707-41-0]	<b>B0639</b> 25g 500g  Isopropyl Bromide [75-26-3]	<b>I0069</b> 25g 100g 500g  Isopropyl Iodide (stabilized with Copper chip) [75-30-9]
<b>D2954</b> 5g 25g  Diisopropyl Sulfate [2973-10-6]	<b>I0914</b> 1g 5g  Isopropyl Methanesulfonate [926-06-7]	<div style="background-color: #4CAF50; color: white; padding: 10px; text-align: center;"> <h3>Butylation &amp; tert-Butylation Reagents</h3> </div>		
	<b>X0039</b> 1set Hydrogen Chloride - Butanol Reagent (5-10%) (1mLx10) [7647-01-0]	<b>X0034</b> 1set Boron Trifluoride - Butanol Reagent (10-20%) (1mLx10) [692-39-7]	<b>O0269</b> 25mL  Tributyl Orthoformate [588-43-2]	
<b>D1302</b> 5mL 25mL  N,N-Dimethylformamide Dibutyl Acetal [18503-90-7]	<b>B0560</b> 25g 500g  Butyl Bromide [109-65-9]	<b>I0055</b> 25g 500g  Butyl Iodide (stabilized with Copper chip) [542-69-8]	<b>D1633</b> 25g 500g  Dibutyl Sulfate [625-22-9]	<b>D1303</b> 5mL 25mL  N,N-Dimethylformamide Di-tert-butyl Acetal [36805-97-7]

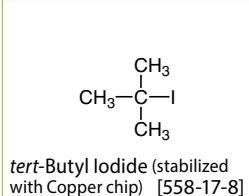
B4178 1g 5g



B0617 25g 100g 500g

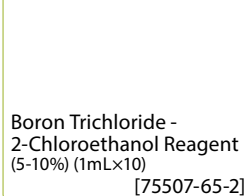


B1072 25g

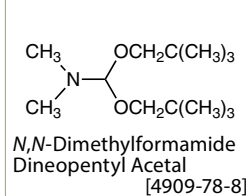


## Other Alkylation Reagents

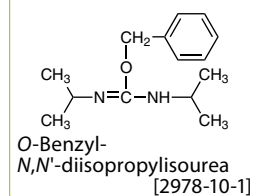
X0032 1set



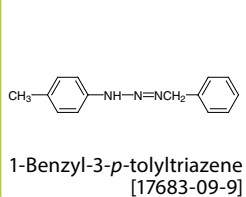
D1595 5mL 25mL



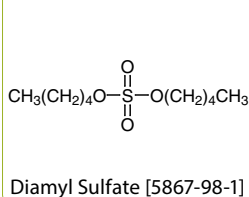
B4480 1mL 5mL



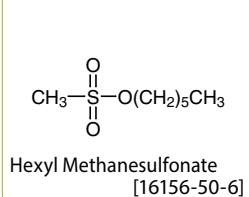
B0949 1g 25g



D2955 5g



H1282 5g 25g



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