

Effects of Branching on Ester Properties

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Background

There are many applications where a low viscosity dry feeling ester is highly desired for use in personal care applications. Low viscosity esters have good spreadability and a cosmetic elegance that is important to applications in skin and sun care.

There are a limited number of options open to the synthetic chemist to make low viscosity esters. They are (a) using low molecular weight reactants, (b) using unsaturated raw materials, (c) using branched raw materials. Examples of products from each class include (a) capryl acetate (b) oleyl oleate and (c) isododecyl isododecanoate. Each type of product has advantageous and disadvantageous. Products from class (a) have a tendency to have malodor and hydrolytic instability issues. Products from class (b) have issues associated with rancidity as the double bond reacts. Products from class (c) are generally expensive.

This paper deals with complex esters of isostearic acid (C18 methyl branched) and isododecanoic acid (C20 long chain branched acid), reacted with polyols to give complex esters.

Complex Esters

Guerbet acid G-20 and Iso-stearic acid (the branched acids) are reacted with the polyhydroxy materials shown below to make the complex esters shown below.

Raw Materials

The Polyols used for this study are shown in Tables 1-3.

Table 1 Neopentyl Glycol	
Structure:	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{-C-CH}_2\text{OH} \\ \\ \text{CH}_2\text{OH} \end{array}$
MW:	136
EMW:	34

Table 2 Trimethylol Propane	
Structure:	$\begin{array}{c} \text{CH}_2\text{OH} \\ \\ \text{CH}_3\text{CH}_2\text{-C-CH}_2\text{OH} \\ \\ \text{CH}_2\text{OH} \end{array}$
MW:	134
EMW:	44.6

Table 3 Pentaerythritol	
Structure:	$\begin{array}{c} \text{CH}_2\text{OH} \\ \\ \text{HOCH}_2\text{-C-CH}_2\text{OH} \\ \\ \text{CH}_2\text{OH} \end{array}$
MW	136
EMW	34

Guerbet Branched Acid (G-20)

Guerbet acids are made by the oxidation of Guerbet alcohols; the structure is shown in table 4.

Table 4 G-20 Guerbet Acid
Structure: $\begin{array}{c} (\text{CH}_2)_7\text{CH}_3 \\ \\ \text{CH}_3-(\text{CH}_2)_9\text{CHCOOH} \end{array}$

Iso-Stearic Acid

Iso-Stearic acid is 16 methyl heptadecanoic acid and is a naturally occurring product conforming to the structure shown in Table 5.

Table 5 Iso-Stearic Acid
Structure: $\begin{array}{c} \text{CH}_3-\text{CH}-(\text{CH}_2)_{14}\text{COOH} \\ \\ \text{CH}_3 \end{array}$

Esterification Reaction

The esterification reaction was run using the ratio of raw materials shown in Tables 6 and 7 using 0.1% stannous oxylate as the catalyst. Water was collected as the reaction proceeded. The reaction was conducted at 200°C for 24 hours.

Table 6

Material	NPG	TMP	PE
Polyol wt.	9.8	12.8	9.80
G-20	90.3	87.2	90.2
Totals	100.0	100.0	100.0

Appearance	Clear liquid	Clear Liquid	Clear liquid
Odor	Mild	Mild	Mild
Color	4	4.6	5
OHV	11	13	13
AV	7	4	3
SAP	163	166	168

Table 7

Material	NPG	TMP	PE
Polyol wt.	10.7	13.5	10.7
Iso-stearic Acid	89.3	86.5	89.3
Totals	100.0	100.0	100.0

Appearance	Clear liquid	Clear liquid	Clear liquid
Odor	Mild	Mild	Mild
Color	2	3	2
OHV	8	13	10
AV	3	4	3
SAP	179	178	181

Results

Table 8 shows the properties of the esters.

Table 8

Properties	TMP G-20	PE G-20	NPG G-20	TMP Isostearate	PE Isostearate	NPG Isostearate
Appearance @ 25 C	Clear	Clear	Clear	Clear	Clear	Clear
Odor	Mild	Mild	Mild	Mild	Mild	Mild
Color, Gardner	4	5	4	3	2	2
Specific Gravity @ 25 C	0.89	0.89	0.88	0.91	0.91	0.91
Viscosity @ 40 C, cSt	73	90	36	105	167	45
Viscosity @ 100 C, cSt	10.3	13	6.6	14	19	7.9
Viscosity Index	126	167	139	138	128	149
Pour Point, C	-50	-45	-40	-26	-18	-35
Flash Point (COC), C	295	298	280	290	290	290
MW	1028	1318	694	930	1198	634

Table 10		
Ester Viscosity		
C-20 G		
NPG	Visc	MW
TMP	36	694
PE	73	1028
	90	1318
Iso-Stearate		
NPG	Visc.	MW
TMP	45	634
PE	105	930
	167	1198

Conclusions

1. The reactions were conducted with no problems producing a clear yellow cosmetically acceptable product.
2. The products made with the Guerbet acid were only slightly darker than esters made with the iso-stearate acid.
3. The iso-stearate esters have lower pour points than the G-20 based products.
4. The viscosity of the esters derived from iso-stearic acid were lower than for those made with the G-20 Guerbet acid.