



Designation: D 2357 – 74 (Reapproved 1995)^{ε1}

Standard for Qualitative Classification of Surfactants by Infrared Absorption¹

This standard is issued under the fixed designation D 2357; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

^{ε1} NOTE—Keywords were added editorially in February 1995.

1. Scope

1.1 This standard covers the qualitative classification of synthetic detergent products or mixtures of synthetic detergents. It is applicable to built detergent formulations as well as individual surfactant compositions.

NOTE 1—The organic active ingredient must be isolated from built syndet compositions in accordance with Test Method D 2358.

1.2 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 2358 Test Method for Separation of Active Ingredient from Surfactant and Syndet Compositions²

3. Summary of Classification

3.1 A portion of the active ingredient is scanned in the infrared region of the spectrum from at least 2 to 15 μm. Qualitative identification of surfactant type is based on the presence of infrared absorption bands attributable to specific functional groups.

3.2 A listing of absorption bands corresponding to the characteristic functional groups of some of the more common types of commercial surfactants is included in this method. Use of available detergent reference spectra may provide additional information.

4. Apparatus

4.1 *Spectrophotometer*, recording, infrared.

4.2 *Dies and Press*, for preparation of KBr disks.

4.3 *Detergent Reference Spectra*.

5. Reagents

5.1 *Mineral Oil*, USP.

5.2 *Potassium Bromide* (KBr), infrared quality, powdered.

5.3 *Additional Reagents*, as specified in Test Method D 2358.

6. Preparation of Sample

6.1 *Sample in Pure Form*—If the sample is in pure form or contains only volatile solvents, dry the sample in accordance with 5.8 of Test Method D 2358, and obtain the infrared spectrum of the dried sample.

6.2 *For Built Surfactants and Synthetic Detergent Compositions*—Obtain the infrared spectrum of the active ingredient(s) separated in accordance with Test Method D 2358.

7. Procedure

7.1 Whenever possible, the infrared spectrum should be obtained directly from the organic material, by formation of a film between salt blocks, and by recording the spectrum between 2 and 15 μm. The film is satisfactory if the spectrum shows 10 to 30 % transmittance in the strongest absorption region.

7.2 If the physical properties of the sample prevent use of the film technique, the spectrum may be made from a mineral oil mull. Form the mull by adding 2 to 3 drops of mineral oil to a small quantity of sample contained in a polished grinding surface (agate) mortar, and grinding for a minimum of 5 min. This should produce a very fine syrupy dispersion. Use the mull as a film between salt blocks and obtain the spectrum as in 7.1.

7.3 If the sample can be obtained in dry, powdered form, the KBr pressed-disk method may be used. Grind the sample sufficiently fine to prevent radiation scatter, and add approximately 1 part sample to 19 parts of dry powdered KBr. Using suitable equipment, form the disk at room temperature in

¹ This classification is under the jurisdiction of ASTM Committee D-12 on Soaps and Other Detergents, and is the direct responsibility of Subcommittee D12.12 on Analysis of Soaps and Synthetic Detergents.

Current edition approved April 29, 1974. Published June 1974. Originally published as D 2357 – 65 T. Last previous edition D 2357 – 69.

² *Annual Book of ASTM Standards*, Vol 15.04.



D 2357

vacuum, under pressure of 10 to 30 tons/in.² Obtain the

spectrum of the disk, sample between 2 and 15 μm as in 7.1.³

8. Identification of Components

8.1 Note the wavelength position of each specific absorption band.

8.2 Identify the absorption bands in terms of functional groups by the use of data in Table 1 or other appropriate reference source.

³ For details of infrared experimental techniques, see Jones, R. N. and Sandorfy, C., "The Application of Infrared and Raman Spectrometry to the Elucidation of Molecular Structure." *Technique of Organic Chemistry*, Vol IX, 1956. Interscience Publishers, Inc., New York, NY.

TABLE 1 Infrared Absorption Bands of Typical Commercial Detergents

Detergent	Wavelength, μm	Frequency, cm ⁻¹	Band Shape ^A	Band Intensity ^B	Identity
Alkylbenzene sulfonate	6.7	1493	shoulder	weak	aromatic bands
	8.1 to 8.5	1235 to 1176	broad ^C	strong	sulfonate group
	8.8	1136	sharp	moderate	sulfonate group
	9.6	1042	sharp	strong	ABS bands
	9.9	1010	sharp	strong	ABS bands
	12.0	833	broad	moderate	para substitution
Fatty alcohol sulfate	8.0	1250	sharp ^D	strong	organic sulfate group
	8.3	1205	sharp ^D	strong	organic sulfate group
	9.2	1087	sharp	moderate	most characteristic alcohol sulfate band
	10.3	971	broad	weak	characteristic alcohol sulfate bands
	10.8	926	broad	weak	characteristic alcohol sulfate bands
Sulfonated amide (taurate)	6.1	1639	sharp	strong	amide carbonyl
	6.4	1563	shoulder	weak	secondary amide
	8.1 to 8.5	1235 to 1176	broad	strong	sulfonate group
	9.4	1064	sharp	strong	C CzN or alkyl sulfonate
Sulfonated ester (isethionate)	5.8	1724	sharp	strong	ester carbonyl
	6.4	1563	broad	weak	soap
	8.1 to 8.5	1235 to 1176	broad	strong	sulfonate group
	8.5	1176	broad	strong	ester C CzO
	9.4	1064	sharp	strong	alkyl sulfonate
Sulfated monoglyceride	3.0	3333	sharp	strong	hindered OH
	5.8	1724	sharp	strong	ester carbonyl
	7.9	1266	sharp ^E	strong	organic sulfate
	8.1	1235	sharp ^E	strong	organic sulfate
	8.5	1176	broad	moderate	ester C CzO
	9.0	1111	broad	weak	H CzC CzOH secondary
	9.4	1064	sharp	moderate	H CzC CzOH secondary
Sulfated phenoxy ether	6.2	1613	sharp	weak	aromatic bands
	6.6	1515	sharp	moderate	aromatic bands
	7.4	1351	broad	weak	polyethylene oxide
	8.0 to 8.2	1250 to 1220	broad	strong	organic sulfate
	8.7 to 9.2	1149 to 1087	broad	strong	polyethylene oxide
	10.5 to 10.9	952 to 917	broad	moderate	polyethylene oxide
	12.0	833	broad	moderate	para substitution
Ethoxylated fatty acid	2.9	3448	sharp	moderate	OH
	5.8	1724	sharp	strong	ester carbonyl
	7.4	1351	sharp	moderate	polyethylene oxide
	8.7 to 9.2	1149 to 1087	broad	strong	polyethylene oxide
	10.5 to 10.9	952 to 917	broad	strong	polyethylene oxide
	8.5	1176	shoulder	moderate	ester C CzO
Ethoxylated fatty alcohol	2.9	3448	sharp	moderate	OH
	7.4	1351	sharp	strong	polyethylene oxide
	8.7 to 9.2	1149 to 1087	broad	strong	polyethylene oxide
	9.4	1064	sharp	moderate	C CzOH
	10.5 to 10.9	952 to 917	broad	strong	polyethylene oxide
Ethoxylated alkyl phenol	2.9	3448	sharp	moderate	OH
	6.2	1613	sharp	moderate	aromatic bands
	6.6	1515	sharp	strong	aromatic bands
	7.4	1351	sharp	strong	polyethylene oxide