# Ionic Mixtures

# Threshold determination for their non-eye irritating properties

## PREAMBLE

Metalworking Fluid concentrates (MWFs) are complex mixtures of chemicals intended to facilitate the various processes in the metal working industry. During the manufacturing process of such MWFs it is unavoidable that some of these chemicals unintentionally react with each other creating new chemicals, which are usually called "Ionic Mixtures" These unintended ionic mixtures cannot be separated from the original mixture and therefore form an intrinsic part of the MWF.

To avoid unnecessary testing of the entire MWF for classification purposes it is important that such properties of the ionic mixtures are also known  By having such data available, the irritation properties of MWF can be calculated in a more appropriate manner and better compared to traditional calculations, which are based on individual added components.

## TEST CONSIDERATIONS AND STATUS

Earlier studies conducted by Boomkamp et al. on behalf of UKLA in 2007 clearly showed that ionic mixtures appear less irritating than its individual components. These studies however did not show clearly where irritating properties changed from irritating into non-irritating properties. All investigations were conducted on concentrated salts or complex mixtures. However, the labelling calculation of the SDS requires data of pure substances. Therefore new studies were carried out in 2014 and 2015, headed by Dr Martin Manikowski on behalf of UEIL. Its goal: Based on a selection of pure ionic mixtures, which were synthesized at laboratory scale, the eye-irritating properties of these ionic mixtures were determined by TNO-Triskelion in Zeist, Netherlands, using the globally accepted method for eye irritation according to OECD 438 (Isolated Chicken Eyes – ICE).

Since it was concluded in 2014 that ionic mixtures, based on MEA or MIPA in combination with acids with a carbon chain length of C14 and higher can be regarded as non-skin irritating substances, the new tests to determine the non-eye irritating properties were conducted on synthesized ionic mixtures using C12, C12-branched, C14, C16 and C18 acids, whilst the bases used were MEA and MIPA.

## TEST RESULTS AND CONCLUSION ON PURE SALTS (100%)

Acids used:

| Mol. Form. | CAS RN | EC Nr | IUPAC Name | Trivial Name | Classification |
|---|---|---|---|---|---|
| C12H24O2 | 143-07-7 | 205-582-1 | Dodecanoic Acid | Lauric Acid | Eye Damage |
| C12H24O2 | 27610-92-0 | 248-570-1 | 2-Butyloctanoic Acid | Butylcaprylic Acid | Eye Irritant |
| C14H28O2 | 544-63-8 | 208-875-2 | Tetradecanoic Acid | Myristic Acid | Eye Irritant |
| C16H32O2 | 57-10-3 | 200-312-9 | Hexadecanoic Acid | Palmitic Acid | Eye Irritant |
| C18H36O2 | 57-11-4 | 200-313-4 | Octodecanonic Acid | Stearic Acid | Non-irritant |

Bases used:

| Mol. Form. | CAS RN | EC Nr | IUPAC Name | Trivial Name | Classification |
|---|---|---|---|---|---|
| C2H7NO | 141-43-5 | 205-483-3 | 2-Aminoethanol | MonoEthanolAmine (MEA) | Eye Damage |
| C3H9NO | 78-96-6 | 201-162-7 | 1-Aminopropan-2-ol | MonoIsoPropanolAmine (MIPA) | Eye Damage |

### Classification overview of ionic mixtures based on acids & bases

| Chain-length | CAS RN of acid | MEA CAS 141-43-5 | MIPA CAS 78-96-6 |
|---|---|---|---|
| C12 | 143-07-7 | **Eye irritant** | **not tested** |
| C12-br. | 27610-92-0 | **Eye damage** | **Eye damage** |
| C14 | 544-63-8 | **Eye irritant** | **Eye Irritant** |
| C16 | 57-10-3 | **non-irritant** | **Eye Irritant** |
| C18 | 57-11-4 | **not tested** | **non-irritant** |

Classifiactions: Eye damage, category 1, H318        Eye irritant, category 2, H139

Based on official tests to date, it can be concluded that the used base influences the non-eye irritating property of the investigated ionic mixtures. The result of the salt MEA with C16 was non-irritant while the result of the salt with MIPA and C16 was eye-irritant. In contrast to the results for non-skin irritating properties, a specific threshold of carbon chain length for non-eye irritating properties could not be determined.

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