ANNEX

PART A

CHEMICAL ACTIVE SUBSTANCES

SECTION 2

Physical and chemical properties of the active substance

2.1. Melting point and boiling point

The melting point or where appropriate the freezing or solidification point of purified active substance shall be determined and reported. Measurements shall be taken up to 360 °C.

The boiling point of purified active substance shall be determined and reported. Measurements shall be taken up to 360 °C.

Where melting point or boiling point cannot be determined because of decomposition or sublimation, the temperature at which decomposition or sublimation occurs shall be reported.

2.2. Vapour pressure, volatility

The vapour pressure of purified active substance at 20 °C or 25 °C shall be reported. Where vapour pressure is less than 10^{-5} Pa at 20 °C the vapour pressure at 20 °C or 25 °C shall be estimated by a vapour pressure curve with measurements at higher temperatures.

In the case of active substances which are solids or liquids, volatility (Henry's law constant) of purified active substance shall be determined or calculated from its water solubility and vapour pressure and be reported (in $Pa \times m^3 \times mol^{-1}$).

2.3. Appearance (physical state, colour)

A description of both the colour, if any, and the physical state of both the active substance as manufactured and purified active substance, shall be provided.

2.4. Spectra (UV/VIS, IR, NMR, MS), molar extinction at relevant wavelengths, optical purity

The following spectra, including a table of signal characteristics needed for interpretation, shall be determined and reported: ultraviolet/visible (UV/VIS), infrared (IR), nuclear magnetic resonance (NMR) and mass spectra (MS) of purified active substance.

Molar extinction at relevant wavelengths shall be determined and reported (ε in $L \times mol^{-1} \times cm^{-1}$). Relevant wavelengths include all maxima in the UV/visible absorption spectrum, as well as the wavelength range of 290-700 nm.

In the case of active substances which are resolved optical isomers, the optical purity shall be measured and reported.

Where necessary for the identification of the impurities considered to be of toxicological, ecotoxicological or environmental significance, the UV/visible absorption spectra, IR, NMR and MS spectra, shall be determined and reported.

2.5. Solubility in water

The water solubility of purified active substances under atmospheric pressure shall be determined and a value reported for 20 °C. These water solubility determinations shall be made in the neutral range (that is to say in distilled water in equilibrium with atmospheric carbon dioxide). If the pKa is between 2 and 12, water solubility shall also be determined in the acidic range (pH 4 to 5) and in the alkaline range (pH 9 to 10). Where the stability of the active substance in aqueous media is such that water solubility cannot be determined, a justification based on test data shall be provided.

2.6. Solubility in organic solvents

The solubility of the active substances as manufactured or purified active substance in the following organic solvents at 15 to 25 °C shall be determined and reported if less than 250 g/L; the temperature applied shall be specified. Results shall be reported as g/L.

(a) Aliphatic hydrocarbon: preferably heptane

(b) Aromatic hydrocarbon: preferably toluene

(c) Halogenated hydrocarbon: preferably dichloromethane

(d) Alcohol: preferably methanol or isopropyl alcohol

(e) Ketone: preferably acetone

(f) Ester: preferably ethyl acetate.

If for a particular active substance, one or more of those solvents is unsuitable (for example reacts with test material), alternative solvents may be used instead. In such cases, choices of solvents shall be justified in terms of their structure and polarity.

2.7. Partition coefficient n-octanol/water

The n-octanol/water partition coefficient (Kow or log Pow) of purified active substance and of all components of the residue definition for risk assessment shall be determined and reported for 20 °C or 25 °C. The effect of pH (4 to 10) shall be investigated when the active substance has a pKa value between 2 and 12.

2.8 Dissociation in water

Where dissociation in water occurs, the dissociation constants (pKa values) of the purified active substance shall be determined and reported for 20 °C. The identity of the dissociated species formed, based on theoretical considerations, shall be reported. If the active substance is a salt the pKa value of the non-dissociated form of the active substance shall be given.

2.9. Flammability and self-heating

The flammability and self-heating of active substances as manufactured shall be determined and reported. A theoretical estimation based on structure shall be accepted if it meets the criteria set out in Appendix 6 of the United Nations' Recommendations on the Transport of Dangerous Goods Manual of Tests and Criteria[(1)]. In justified cases, data for purified active substance may be used.

2.10. Flash point

The flash point of active substances as manufactured with a melting point below 40 °C shall be determined and reported. In justified cases, data for purified active substance may be used.

2.11. Explosive properties

The explosive properties of active substances as manufactured shall be determined and reported. A theoretical estimation based on structure shall be accepted if it meets the criteria set out in Appendix 6 of the United Nations 'Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria'. In justified cases, data for purified active substance may be used.

2.12. **Surface tension**

The surface tension of purified active substance shall be determined and reported.

2.13. **Oxidising properties**

The oxidising properties of active substances as manufactured, shall be determined and reported. A theoretical estimation based on structure shall be accepted if it meets the criteria set out in Appendix 6 of the United Nations 'Recommendations on the Transport of Dangerous Goods Manual of Tests and Criteria'. In justified cases data for purified active substance may be used.

2.14. **Other studies**

Supplementary studies necessary for the classification of the active substance by hazard shall be carried out in accordance with Regulation (EC) No 1272/2008.

(**1**) United Nations New York and Geneva (2009) Publication ISBN 978-92-1-139135-0.

Changes to legislation:
There are outstanding changes not yet made to Commission Regulation (EU) No 283/2013. Any changes that have already been made to the legislation appear in the content and are referenced with annotations.
View outstanding changes

Changes and effects yet to be applied to the whole legislation item and associated provisions

- Signature words omitted by S.I. 2019/556 reg. 21(4)
- Annex Pt. A s. 8 word omitted by S.I. 2019/556 reg. 21(5)(b)(xiv)
- Annex Pt. A s. 1 point 1.4 word substituted in earlier amending provision S.I. 2019/720, Sch. 2 para. 176(2)(a)(i) by S.I. 2020/1567 Sch. 2 para. 61
- Annex Pt. A s. 1 point 1.4.1 word substituted in earlier amending provision S.I. 2019/720, Sch. 2 para. 176(2)(b) by S.I. 2020/1567 Sch. 2 para. 61
- Annex Pt. B s. 9 words omitted by S.I. 2019/556 reg. 21(5)(c)(vi)
- Art. 1(1) Art. 1 renumbered as Art. 1(1) by S.I. 2019/556 reg. 21(2)(a)
- Art. 1(2) inserted by S.I. 2019/556 reg. 21(2)(b)