



Draft Assessment Report

Evaluation of Active Substances

Plant Protection Products

Prepared according to **Regulation (EC) 1107/2009**
as it applies in Great Britain

Elemental iron

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Great Britain

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B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.1. MELTING POINT AND BOILING POINT						
Melting, freezing or solidification point B.2.1/01	Peer reviewed literature	Iron (pure active substance)	Melting point: 1535 °C	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	N	CA 2.1/01: Weast, R. C. (1983) CRC Handbook of Chemistry and Physics 64th Edition. p. B-18 – B19.
Boiling point B.2.1/02	Peer reviewed literature	Iron	Boiling point: 2750°C	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	N	
Decomposition / Sublimation temperature B.2.1/03	-	-	Not determined.	Not considered necessary as the melting point and boiling point were able to be determined; decomposition and sublimation did not occur.	-	-
B.2.2. VAPOUR PRESSURE, VOLATILITY						
Vapour pressure B.2.2/01	-	-	Elemental iron is an inorganic solid with negligible volatility under ambient conditions. Non-volatile.	Acceptable.	-	-
Volatility (Henry's Law constant) B.2.2/02	Quotient of vapour pressure and water solubility	-	A Henry's law constant is not applicable since iron is not volatile and is insoluble in water.	Acceptable.	-	-
B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)						
Physical state and colour B.2.3/01	-	Iron powder (pure active substance)	Silvery-white or grey lustrous powder	Acceptable.	N	CA 2.3/01: Windholz, M. (1983), The Merck Index - An Encyclopaedia of

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
		Elemental iron technical material Batch 2290598 (98.0%)	Powdered solid, grey without odour (at 21°C)		Y	Chemicals, Drugs, and Biologicals, 10th edition, p. 4944. CA 2.9/01: [REDACTED] (2018), Mo5844.
B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY						
Ultraviolet/visible (UV/VIS) B.2.4/01	-	-	An UV/Vis absorption spectrum is not relevant since iron is insoluble in water.	Acceptable.	-	-
Infrared (IR) B.2.4/02	-	-	An IR spectrum is not relevant since it is not characteristic for iron	Acceptable.	-	-
Nuclear magnetic resonance (NMR) B.2.4/03	-	-	A NMR spectrum is not relevant since iron does not have an NMR active nucleus.	Acceptable.	-	-
Mass spectra (MS) B.2.4/04	-	Elemental iron technical material	An MS spectrum for iron is not relevant. As an element no diagnostic fragmentation pattern is possible. Elemental iron consists of four stable isotopes, ⁵⁴ Fe, ⁵⁶ Fe, ⁵⁷ Fe and ⁵⁸ Fe, with average natural abundances of ~6%, 92%, 2% and <1%. An ICP-MS pattern would be expected to provide signals which align with these masses at the respective distribution levels. Representative ICP optical emission spectra generated using the technical material show characteristic peaks when analysed at a wavelength of 273.955 nm.	Acceptable.	-	-
Spectra for impurities B.2.4/05	-	Elemental iron technical material	Impurities in elemental iron are likewise metallic elements for which spectral information are not diagnostic as discussed for iron itself.	Acceptable.	-	-

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
			<p>Arsenic: Representative ICP optical emission spectra generated using the technical material show characteristic peaks when analysed at a wavelength of 200.334 nm.</p> <p>Lead: Analysis of the technical material using Graphite Furnace Atom Absorption Spectroscopy at two wavelengths (283.3 and 217.0 nm), showing characteristic spectra.</p> <p>Mercury: Representative AFS (Atomic Fluorescence Spectroscopy) spectra generated using the technical material show characteristic peaks using this method which is highly specific to the element mercury.</p> <p>Cadmium: Representative ICP optical emission spectra generated using the technical material show characteristic peaks when analysed at a wavelength of 228.802 nm.</p> <p>Nickel: Representative ICP optical emission spectra generated using the technical material show characteristic peaks when analysed at a wavelength of 231.604 nm.</p>			
B.2.5. SOLUBILITY IN WATER						
Solubility in water B.2.5/01	Peer reviewed literature	Iron	Elemental iron is insoluble in water	<p>Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.</p> <p>The MSDS provided for 'elemental iron powder' states a water solubility of 0.015 mg/L at 22°C. (Note: the solubility increases at the acidity in water increases). This is very low value and supports the information available in the peer reviewed literature. The note regarding change in solubility with pH has not been considered further as this is not critical to the environmental risk assessment.</p>	N	CA 2.5/01: Weast, R. C. (1983) CRC Handbook of Chemistry and Physics 64th Edition. p. B-99.
B.2.6. SOLUBILITY IN ORGANIC SOLVENTS						

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
Solubility in organic solvents B.2.6/01	Peer reviewed literature	Iron	Elemental iron is insoluble in organic solvents.	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	N	CA 2.6/01: Weast, R. C. (1983) CRC Handbook of Chemistry and Physics 64th Edition p. B-99.
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER						
Partition coefficient n-octanol/water B.2.7/01	-	-	Not relevant as iron is not soluble in water or organic solvents. As iron is the only component of the residue definition, no further consideration is required.	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	-	-
B.2.8. DISSOCIATION IN WATER						
Dissociation constant B.2.8/01	-	-	Not relevant since iron is not soluble in water.	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	-	-
B.2.9. FLAMMABILITY AND SELF-HEATING						
Flammability B.2.9/01	EC Method A10	Elemental iron technical material Batch 2290598 (98.0%)	The test item could not be ignited by a flame within 5 minutes. Therefore the main test was not necessary. The test item is not a highly flammable solid in the sense of Reg (EU) No. 440/2008.	Acceptable.	Y	CA 2.9/01: (2018), Mo5844.
Self heating B.2.9/02	EC Method A16	Elemental iron technical material Batch 2290598 (98.0%)	A self-ignition temperature of 365°C was observed.	Acceptable.	Y	CA 2.9/02: (2017), PS20170427-2.
B.2.10. FLASH POINT						

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
Flash point B.2.10/01	-	-	Not required for solids. Additionally, melting point is >60°C.	Acceptable. Not required for a solid active substance.	-	-
B.2.11. EXPLOSIVE PROPERTIES						
Explosive properties B.2.11/01	EC Method A14 and OECD 113	Elemental iron technical material Batch 2290598 (98.0%)	The test substance did not exhibit explosive properties when subject to thermal and mechanical stresses.	Acceptable.	Y	CA 2.11/01: (2017a), PS20170427-1.
B.2.12. SURFACE TENSION						
Surface tension B.2.12/01	-	-	Not relevant since iron is not soluble in water.	Acceptable. Published literature provided by the applicant is considered sufficient to address this data requirement as a range of published peer reviewed literature is available containing information about elemental iron.	-	-
B.2.13. OXIDISING PROPERTIES						
Oxidizing properties B.2.13/01	-	-	Not oxidising. In accordance with Appendix 6 of the United Nations 'Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria', for inorganic substances, such as elemental iron, the test procedures need not be applied as the substance does not contain any oxygen or halogen atoms. Therefore the active substance is not considered oxidising.	Acceptable.	-	-
B.2.14. OTHER STUDIES						
Density	Peer reviewed literature	Iron	The density of iron is 7.86 g/cm ³ .	This property is not required by the Regulation therefore has not been considered further and has been reported for completeness.	-	CA 2.14/01: Weast, R. C. (1983) CRC Handbook of Chemistry and Physics 64th

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
						Edition. p. B-99.

Elemental Iron Pure Active Ingredient

Elemental iron is a grey powder. It has a melting point of 1535°C and a boiling point of 2750°C. Elemental iron is not soluble in water therefore properties such as vapour pressure, Henry's law constant, dissociation constant and surface tension were not applicable. Elemental iron is also not soluble in organic solvents. UV/Vis, IR, NMR and MS spectra data were not provided as these techniques are not appropriate for the determination of elemental iron. Highly specific techniques such as ICP-OES are available for the determination and identification of elemental iron. Elemental iron is not flammable, oxidising or explosive.

Elemental Iron Technical Grade Active Ingredient

Elemental iron is a grey powder with no odour. It has a melting point of 1535°C and a boiling point of 2750°C. Elemental iron is not soluble in water therefore properties such as vapour pressure, Henry's law constant, dissociation constant and surface tension were not applicable. Elemental iron is also not soluble in organic solvents. UV/Vis, IR, NMR and MS spectra data were not provided as these techniques are not appropriate for the determination of elemental iron. Highly specific techniques such as ICP-OES are available for the determination and identification of elemental iron. Elemental iron is not flammable, oxidising or explosive.

B.2.15. REFERENCES RELIED ON

Data Point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evaluation
B2.1/01, B2.5/01, B2.6/01, 2.14/01	Weast, R. C. (editor)	1983	CRC Handbook of Chemistry and Physics 64th Edition, CRC Press. p. B-18 – B19. N/A GLP: No Published: Yes	N	N	-	Publish ed Literat ure	N/A
B2.3/01	Windholz, M. (editor)	1983	The Merck Index - An Encyclopaedia of Chemicals, Drugs, and Biologicals, 10th edition, p. 4944. N/A GLP: No Published: Yes	N	N	-	Publish ed Literat ure	N/A
B2.3/01, B2.9/01		2018	Determination of physico- chemical properties for elemental iron powder BioGenius GmbH Mo5844 GLP: Yes Published: No	N	Y	Article 59(1) & (2) of Regulation (EC) 1107/2009 applies.	ADA MA	N/A
B2.9/02		2017	Elemental iron powder Batch No.:2290598 AUTO- FLAMMABIL ITY (SOLIDS- DETERMINA TION OF RELATIVE SELF- IGNITION TEMPERATU RE) A.16	N	Y	Article 59(1) & (2) of Regulation (EC) 1107/2009 applies.	ADA MA	N/A

Data Point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evaluation
			Siemens Prozess- Sicherheit PS20170427-2 GLP: Yes Published: No					
B2.11/01		2017	Elemental iron powder Batch No.:2290598 EXPLOSIVE PROPERTIES A.14 Siemens Prozess- Sicherheit PS20170427-1 GLP: Yes Published: No	N	Y	Article 59(1) & (2) of Regulation (EC) 1107/2009 applies.	ADA MA	N/A
B2.13/01	United Nations	2009	Recommendati ons on the Transport of Dangerous Goods Manual of Tests and Criteria, 5th revised edition N/A GLP: No Published: Yes	N	N	-	Publish ed Literat ure	N/A