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Sect	ion A3	Physical and Chen	nical Properties	of Active Substance					
	Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only
3.1	Melting point, boiling point, relative density (IIA3.1)								
3.1.1	Melting point	EEC Directive 92/69 EEC A.1 (DSC)	Not indicated	<- 90 °C During a DSC experiment, the substance was cooled down to -90 °C without solidification.	According to the TNsG on data requirements "Usually the freezing point of liquid substances should be determined if above -20°C. An indication that no freezing has occurred during preliminary tests is also acceptable." Therefore, the applicant considers the performed study as sufficient to cover this data requirement and the performance of a GLP test not to be necessary.	N		112-002 A3.1.1/01	X

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	Subsection (Annex Point)	Method	Purity/ Specification	Results  Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only
3.1.2	Boiling point	EEC Directive 92/69 EEC A.2 EPA OPTTS 830.7220 EPA subdivision D series 63-6	purity: 99.8%	- exothermic effect at ca. 141 °C (probably decomposition) - endothermic effect slightly below 300 °C (metastable boiling point)	Differential Scanning Calori- meter (DSC) was used	Y	miles:	112-001 A3.1.2/01	x
3.1.3	Bulk density/ relative density								
	rel. density	EEC Directive 92/69 EEC A,3 OECD 109 EPA OPTTS 830.7300 EPA subdivision D series 63-7	purity: 99.8%	0.998 (at 20°C +/- 0.5 °C)	Measured with a pycnometer	Y		113-001 A3.1.3/01	*
3.2	Vapour pressure (IIA3.2)	EEC Directive 92/69 EEC A.4 (static technique). OECD 104 EPA OPTTS 830.7950 EPA subdivision D series 63-9	purity: 99.8%	0.15 +/- 0.01 Pa at 20°C 0.22 +/- 0.01 Pa at 25°C	None. Calculated via Inp/T <sup>-1</sup> curve: In p [Pa] = -6874.6/T[K] + 21.548	Y	į	115-001 A3.2/01	

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3.2.1	Henry's Law Constant (Pt. I-A3.2)	Calculated parameter	Not applicable	0.000461 Pa m <sup>3</sup> mol <sup>-1</sup> (20°C)	Calculated with reference to: Aqueous solubility = 70 g/L (20°C) (see 3.5) Vapour pressure = 0.15 Pa (20°C) (see 3.2) Molar weight = 215.29 g/mol	N		None	
3.3	Appearance (IIA3.3)								
3.3.1	Physical state	EPA OPPTS 830.6303 EPA subdivision D series 63-3	purity: 99.8%	Liquid (at 21°C)	None	Y		111-001 A3.3.1/01	
3.3.2	Colour	EPA OPPTS 830.6302 EPA subdivision D series 63-2	purity: 99.8%	Clear and colourless (at 21°C)	None	Y	a da	111-001 A3.3.1/01	
3.3.3	Odour	EPA OPPTS 830.6304 EPA subdivision D		No characteristic odour (at 21°C)	None	Y		111-001 A3.3.1/01	

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## Physical and Chemical Properties of Active Substance Section A3 Subsection Method Purity/ Results Reliability Official Remarks/ GL Reference (Annex Point) Specification Justification P use Give also data on test (Y/ only pressure, temperature, pH N) and concentration range if necessary Absorption spectra (IIA3.4) OECD 101 None 117-001 No absorbance maxima 3.4.1 UV/VIS EPA OPTTS 830,7050 were observed under A3.4.1/01 purity: 99.8% neutral (900 - 200nm), acidic (900 - 205nm) and alkaline conditions (900 -220nm) (25°C +/ 0.5 °C) No guideline Not mentioned The respective spectra None N 117-002 mentioned confirms the molecular A3.4.1/02 structure of IR3535 50,08 mg in 50 mL The UV-VIS spectrum None 117-003 water. 200 - 800 nm. shows only the flank of A3.4.1/03 Slit 2 nm. Intervall 0.1 purity: 99.4% the absorption bands due s. Stepsize 0.5 nm. to n $\rightarrow \pi^*$ transitions of Base line: water. Cell the ester and amide group length: 1 cm. below 250 nm. No guideline Not mentioned The respective spectra None N 117-002 3.4.2 IR mentioned confirms the molecular A3.4.1/02 structure of IR3535 FT-IR Spectroscopy, The respective spectrum None 117-003 Bruker Vector 22, confirms the molecular A3.4.1/03 spectral resolution purity: 99.4% structure of IR3535 2 cm<sup>-1</sup>, 32 scans, KBr-No guideline Not mentioned The respective spectra None 117-002 3.4.3 NMR mentioned confirms the molecular A3.4.1/02

structure of IR3535

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CF CF		Bruker DPX300; samples in d <sub>6</sub> -DMSO, <sup>1</sup> H: 353K, 32 scans <sup>13</sup> C: 393K, 1024 scans	purity: 99.4%	The respective spectra confirm the molecular structure of IR3535	None	N		117-003 A3.4.1/03	
3.4.4	MS	No guideline mentioned	Not mentioned	The respective spectra confirms the molecular structure of IR3535	None	N	į.	117-002 A3.4.1/02	
		EI-MS. Waters "Autospec" at 140 °C.	purity: 99.4%	The respective spectrum confirms the molecular structure of IR3535	None	N		117-003 A3.4.1/03	,
3.5	Solubility in water (IIA3.5)								
	Water solubility	EEC Directive 92/69 EEC A.6 OECD 105 EPA OPTTS 830.7840 EPA subdivision D series 63-8	purity: 99.8%	70 g/L at 20.0°C +/- 0.5°C	Shake flask method, using distilled water, without pH control was used.	Y	in the second	114-004 A3.5/01	

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	Subsection (Annex Point)	Method	Purity/ Specification	Results  Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only
	Water solubility	EEC Directive 92/69 EEC A.6	purity: 99.9%	pH 5: 69.92 g/L pH 7: 56.72 g/L pH 9: 68.0 g/L (t 20°C +/- 1°C)	Shake flask method was used. At pH 9 the test item was unstable due to hydrolysis. The given result is assumed to reflect the equilibrium between hydrolysis and solubility.	Y		114-005 A3.5/02	
3.6	Dissociation constant (-)			Not applicable	The test item is not ionisable and therefore could not dissociate in water. A detailed justification is provided in the "Evaluation by Competent Authorities" table at the end of this document.				
3.7	Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	EPA subdivision D series 63-8	purity: 99.8%	Acetone >1000g/L Ethyl acetate >1000g/L Dichloromethane >1000g/L n-Heptane >1000g/L Methanol >865g/L p-Xylene >1000g/L	None	Y		114-001 A3.7/01	

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## Section A3 Physical and Chemical Properties of Active Substance Subsection Method Purity/ Results GL Reliability Reference Official Remarks/ (Annex Point) Specification Justification P use Give also data on test (Y/ only pressure, temperature, pH N) and concentration range if necessary (at room temperature) 114-001 Stable in common organic Additional 3.8 Stability in organic solvents information A3.7/01 solvents used in b.p. confirming the and identity of stability of IR3535® 114-006 relevant breakdown in the organic A3.8/01 products solvent ethanol that (IIIA3.2) is mostly used in formulation is given in Doc-no.: 114-006 This document contains confidential information and therefore notifier requests a confidential treatment of this document. 3.9 Partition coefficient n-octanol/water (IIA3.6) log Pow HPLC method 114-003 EEC Directive log Pow: 1.7 92/69 EEC A.8 As the test item is A3.9/01 (at: 23-24°C) **OECD 117** purity: 99.8% not ionisable, investigation on the EPA OPTTS 830,7570 pH effect on the EPA subdivision D series 63-11 partition coefficient

is not necessary.

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## Section A3 Physical and Chemical Properties of Active Substance Subsection Method Purity/ Results GL Reliability Reference Official Remarks/ (Annex Point) Specification Justification P use Give also data on test (Y/ only pressure, temperature, pH N) and concentration range if necessary 141-001 CIPAC MT 46 The test substance is No changes in its 3.10 Thermal stability, EPA OPTTS 830.6313 stable at 54 °C for 14 purity was A3.10/01 identity of relevant EPA subdivision D purity: 99.8% days. measured. No breakdown products breakdown products series 63-13 No exothermal decom-(IIA3.7) position was observed up were identified. to 141 °C, please refer to 3.1.2 3.11 Flammability, including autoflammability and identity of combustion products (IIA3.8) Not applicable According to TNsG Flammability the flammability of substances which are solids, gases or substances which evolve highly flammable gases must be determined. This is not the case for IR3535® a testing is therefore not necessary. Not auto-flammable No exothermal **Auto-flammability**

decomposition was

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	Subsection (Annex Point)	Method	Purity/ Specification	Results  Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only
i.e					observed up to 350 °C, please refer to 3.1.2				
3.12	Flash-point (IIA3.9)	EEC Directive 92/69 EEC A.9 DIN EN22719 EPA OPTTS 830.6315 EPA subdivision D series 63-15	purity: 99.8%	159°C	Pensky Martens closed cup	Y		142-001 A3.12/01	
3.13	Surface tension (IIA3.10)	EEC Directive 92/69 EEC A.5	purity: 99.7%	59.6mN/m at 20.0°C ± 0.5°C (n=3)	Ring method concentration of test solution: 1 g/L aqueous solution	Y		116-002 A3.13/01	
3.14	Viscosity (-)	OECD 114 DIN 53019 Teil 1 EPA OPTTS 830.7100 EPA subdivision D series 63-18	purity: 99.8%	Viscosity: $14 - 22$ mPa.s (at $20^{\circ}\text{C} \pm 0.5^{\circ}\text{C}$ ) Viscosity: $16$ mPa.s at $(40^{\circ}\text{C} \pm 0.4^{\circ}\text{C})$	Rotational Viscometer	Y		116-001 A3.14/01	
3.15	Explosive properties (IIA3.11)	EEC Directive 92/69 EEC A.14	Not applicable	Not explosive	The compound does not contain reactive groups that indicates explosive properties.	N	2 d	141-003 A3.15/01	
		Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods,	Not applicable	Not explosive  Based on a screening of the molecular structure of IR3535 according to	A detailed justification is provided in the "Evaluation by Competent	N			3 3

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Section A3	Physical and Chemical Properties of Active Substance									
Subsection (Annex Point)	Method	Purity/ Specification	Results  Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only		
	Manual of Tests and Criteria"(4 <sup>th</sup> revised edition)		Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria", it can reasonably be concluded that IR3535 is not explosive.	Authorities" table at the end of this document.						

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3.16	Oxidising properties (IIA3.12)	EEC Directive 92/69 EEC A.17	Not applicable	Not oxidising	The compound does not contain reactive groups that indicates oxidising properties.	N		141-003 A3.15/01		
		Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria" (4 <sup>th</sup> revised edition) and supplement to A.17	Not applicable	Not oxidising Based on the criteria set out in the Appendix 6 of the United Nations "Recommendations on the Transport of Dangerous goods, Manual of Tests and Criteria" (4th revised edition) and the criteria set out in the supplement to A.17* method as provided by the UK Health and Safety Executive (http://www.hse.gov.uk/nons/nonsa17.htm) it can reasonably be concluded that IR3535 is not oxidising.	A detailed justification is provided in the "Evaluation by Competent Authorities" table at the end of this document.	N				

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## Section A3 Physical and Chemical Properties of Active Substance Subsection (Annex Point) Method Purity/ Specification Give also data on test

	Subsection (Annex Point)	Method	Purity/ Specification	Results  Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GL P (Y/ N)	Reliability	Reference	Official use only
3.17	Reactivity towards container material (IIA3.13)	EPA OPTTS 830.6313 EPA subdivision D series 63-13	purity: 99.8%	No significant change in appearance and/or decrease in concentration was observed after exposition of IR3535® to iron/iron ions and copper/copper ions for 14 days at 20°C ± 1°C and 54°C ± 1°C, respectively.	None	Y	er 19	146-001 A3.17/01	
		EPA OPTTS 830.6317 EPA OPTTS 830.6320	purity: 99.8 %	The commercial storage container (HDPE) does not change physically during a 1 year storage period at warehouse conditions.	None	Y		146-003 A3.17/02	

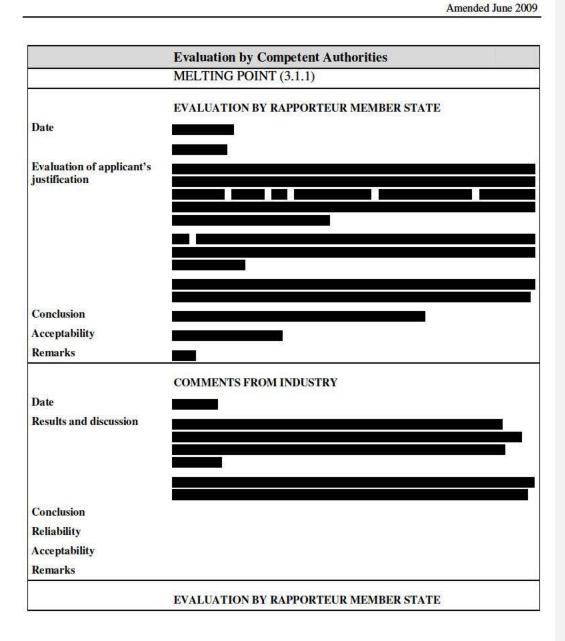
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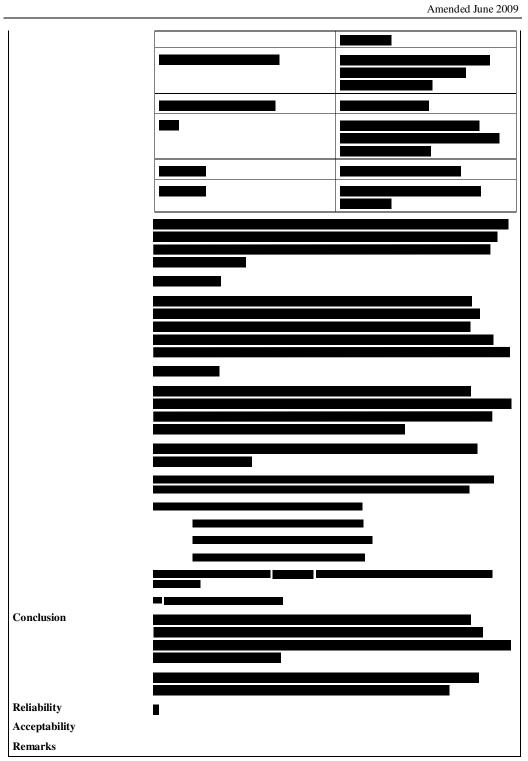
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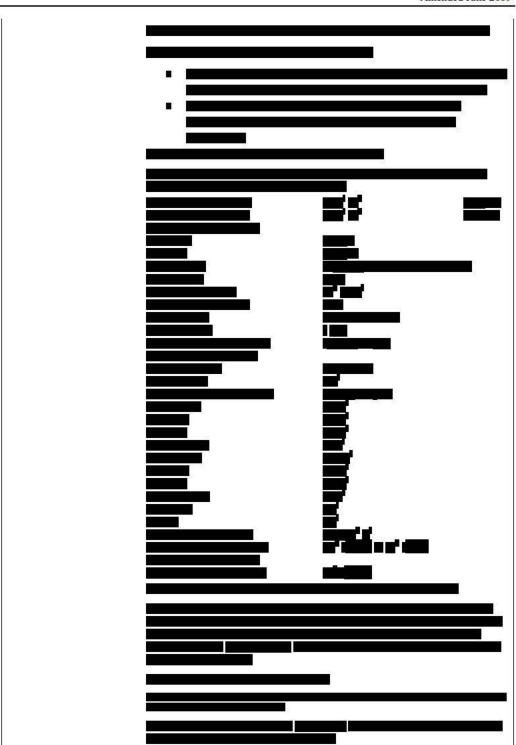
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