European Commission

TRANSFLUTHRIN

CAS number 118712-89-3

Document III-A
Section 3 Physical and Chemical Properties
Study Summaries
Active Substance

Rapporteur Member State: The Netherlands
August 2013

CA-report and Proposed Decision of The Netherlands in the context of the
Possible inclusion of Transfluthrin in Annex I of Council Directive 98/8/EC

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Section A3	Physical and Chemical Properties of Active Substance							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Differential scanning calorimetry in accordance with OECD Guideline 102	Batch No. EATFTJ005, 99.1% (w/w)	32ºC		Y	1	Smeykal, H (2005), Transfluthrin (Bayothrin), NAK 4455; Substance, Technical AE 003547 00 1D99 0004: Melting Pont (OECD 102) ; Thermal Stability (OECD 113), Siemens AG, Prozess-Sicherheit, Report No. 20050216.01 BES Ref: M-254400-01-1 30.05.05 GLP. unpublished	X
3.1.2 Boiling point	Siwoloboff method in accordance with OECD Guideline 103 and EEC A 2	Batch No. 91031ELB01, 98.0% (w/w)	242ºC at 1033 hPa		Y	1	Krohn, J (1991), Boiling Point of NAK 4455 Bayer AG, Business Group Crop Protection, Report No. 14 150 0724 BES Ref: MO-04-012197 10.12.91 GLP. unpublished	

Continued

Section A3	**Physical and Chemical Properties of Active Substance**							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.1.3 Bulk density/ relative density	Flexual resonator method using the density meter DMA 38, based on EPA OPPTS 830.7300, DIN 51757 procedure D, EC A.3, and OECD guideline 109	Batch No. EATFTJ005, 99.1% (w/w)	1.3856 g/cm^3 at 20ºC 1.3624 g/cm^3 at 40ºC		Y	1	Rexer, K and Bittner, P (2005), Physical, Chemical and Technical Properties of Transfluthrin, Bayer CropScience GmbH Report No. WIR0132 (PC) 01 BES Ref: M-253445-01-1 02.06.05 GLP, unpublished	X
3.2 Vapour pressure (IIA3.2)	Gas saturation method in accordance with OECD Guideline 104.	Batch No. APF11088650, purity 97.8 %	**Temp** / **Vapour pressure** 20 °C: 9x10^{-4} Pa 25 °C: 2x10^{-3} Pa	Vapour pressures extrapolated from measurements between 30°C and 85 °C.	Y	1	Weber, R and Krohn, J (1995), Vapour Pressure Curve of NAK 4455, Bayer AG Report AP No. 682 260. 20.09.95 GLP. Unpublished	X
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	Calculated from water solubility and vapour pressure.		**Calculated:** 5.86 Pa m^{3}mol^{-1} at 20ºC 13 Pa m^{3}mol^{-1} at 25ºC	Calculated using data from points 3.2 and 3.5	Y	1	Bogdoll, B and Lemke, G (2005), Henry's Law Constant of Transfluthrin, NAK 4455 (AE 0035474) Bayer CropScience GmbH Report No. AF05/041; BES Ref: M-254216-01-1. 14.07.05 GLP. Unpublished	X

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Section A3 Physical and Chemical Properties of Active Substance								
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.3 Appearance (IIA3.3)								
3.3.1 Physical state **3.3.2 Colour** **3.3.3 Odour**	EPA OPPTS 830.6302, 830.6303, 830.6304 and Directive 94/37/EC (Annex 1; 2.4)	Pure substance batch M22558, 99.3% (w/w) Technical batch EATFTJ005, 99.1% (w/w)	Pure substance: crystalline, white needles; no characteristic odour Technical: off-white needles; toluene-like odour		Y	1	Bogdoll, B and Eyrich, U (2005), Physical Characteristics Color, Appearance and Odor of Transfluthrin, Bayer CropScience GmbH, Report No. PA05/010; BES Ref: M-254180-01-1 02.06.05 GLP, unpublished	
3.4 Absorption spectra (IIA3.4)								
UV/VIS	Spectrophotometric method – in-house. Perkin-Elmer spectrophotometer 554 was used. A range of solutions of the test substance with nominal concentration of 6.156×10^{-2} mg/ml were prepared and scanned between 200 nm and 375 nm using a methanol reference.	Batch No. APF 04118650 Purity: 98.4%	The peak maximum is at 210 nm		N	1	Krohn, J (1987), NAK4455 UV-Vis Spectrum. Bayer AG Report PF-F.CE/QS 1 BES Ref: M0-99-015149 10.03.87 Non-GLP Unpublished	X

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Section A3	**Physical and Chemical Properties of Active Substance**							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
IR	Infrared spectrometry, in-house method. KBr-Preβling; Operating scan range 4000-500 cm^{-1}.	Batch No. APF 04118650 Purity: 98.4%	**Stretch Absorbance** alkene 3080 aliphatic 2988 C=O 1737 Aromatic 1506  1391 C-O-C 1177 $Cl_2C=CH$ 915 The spectrum is consistent with the proposed structure of Transfluthrin		N	1	Krohn, J (1987), NAK4455 UV-Vis Spectrum. Bayer AG Report PF-F.CE/QS 1 BES Ref: M0-99-015149 10.03.87 Non-GLP Unpublished	X
NMR	Nuclear Magnetic Resonance spectrometry, in-house method. Spectra were obtained using a Bruker, Model AM 250 NMR spectrometer. Operating frequency 62,89 MHz (carbon) or 250 MHz (proton).	Batch No. APF 04118650 Purity: 98.4%	The spectrum is consistent with the proposed structure of Transfluthrin		N	1	Krohn, J (1987), NAK4455 UV-Vis Spectrum. Bayer AG Report PF-F.CE/QS 1 BES Ref: M0-99-015149 10.03.87 Non-GLP Unpublished	X

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Section A3	Physical and Chemical Properties of Active Substance							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
MS	Mass Spectrometry in accordance with in-house method. Spectra were obtained by GC-MS using a HP 5987 MS detector	Batch No. APF 04118650 Purity: 98.4%	The spectrum is consistent with the proposed structure of Transfluthrin.		N	1	Krohn, J (1987), NAK4455 UV-Vis Spectrum. Bayer AG Report PF-F.CE/QS 1 BES Ref: M0-99-015149 10.03.87 Non-GLP Unpublished	X
3.5 Solubility in water (IIA3.5)	Column elution method in accordance with OECD Guidelines No. 105.	Batch APF11088650. Purity, 97.8%	result: 0.057 ± 2.94 mg/L temperature: 20 °C		Y	1	Krohn, J (1995) Water Solubility of NAK 4455, Bayer AG Report No. 5/0124. BES Ref: MO-03-010371 29.09.95 GLP, Unpublished.	X
3.6 Dissociation constant (-)	Titration, spectrophotometric, and conductometric methods in accordance with OECD Guideline 112		Nor applicable since the chemical structure of transfluthrin does not contain any acidic protons or basic centres; therefore, no dissociation in water occurs.	All methods not applicable due to low water solubility (57 µg/L at 20ºC.	Y	1	Bogdoll, B and Lemke, G (2005), Transfluthrin, NAK 4455: Statement on the Dissociation Constant, Bayer CropScience GmbH, Report No. AF05/009 BES Ref: MO-05-0073464, 14.04.05 GLP. Unpublished	X

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Section A3	**Physical and Chemical Properties of Active Substance**							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Direct addition method in accordance with OECD guideline 105 and EEC A.6	Batch No. EATFTJ005, 99.1% (w/w)	Solubility at 20ºC: Ethanol ~1.6 kg/L n-Hexane 5 -6.7 kg/L Toluene 6.7-10 kg/L Dichloro-methane 10-20 kg/L Acetone 10-20 kg/L Ethyl acetate 6.7-10 kg/L Dimethyl-sulfoxide 6.7-10 kg/L		Y	1	Bogdoll, B and Eyrich, U (2005), Solubility of Transfluthrin NAk 4455 (AE 0035474) in Organic Solvents, Bayer CropScience GmbH, Report No. PA05/009 ; BES Ref: M-254129-01-1 02.06.05 GLP. Unpublished	X
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)			Not applicable					
3.9 Partition coefficient n-octanol/water (IIA3.6)	Shake flask method in accordance with OECD-Guidelines No. 107	Batch APF11088650. Purity, 97.8%	result: log Pow = 5.46 temperature: 20ºC		Y	1	Krohn, J (1995). Partition Coefficient of NAK 4455 Bayer AG Report No. 5/0125 BES Ref: M0-03-011157 29.09.95 GLP Unpublished	X

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Section A3 Physical and Chemical Properties of Active Substance								
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	Differential scanning calorimetry in accordance with OECD Guideline 113	99.1% (w/w), Batch No. EATFTJ005	Endothermic effect (melting) at a temperature of about 30ºC and an exothermal decomposition in the temperature range 250-390ºC with a maximum energy of 618 J/g	Graphical presentations included in report	Y	1	Smeykal, H (2005), Transfluthrin (Bayothrin), NAK 4455; Substance, Technical: Melting Point (OECD 102) ; Thermal Stability (OECD 113), Siemens AG Prozess-Sicherheit Report No. 20050216.01 BES Ref: M-254400-01-1 30.05.05 GLP. unpublished	X
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	Investigated as stipulated in DIN 51794 and EC Guideline A 15.	Batch No. 816779502, Purity: 95.7%	Auto-ignition temperature = 415ºC		Y	1	Heitkamp, D (2001), Determination of Safety-Relevant Data of NAK 4455 techn, Bayer AG Report No. 01/00146 BES Ref: M0-03-010048 12.04.01 GLP. Unpublished	

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Section A3	**Physical and Chemical Properties of Active Substance**							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.12 Flash-point (IIA3.9)	Investigated as stipulated in EC test procedure A 9	Batch No. EATFTJ005, 99.1% (w/w)	Flash point = 119.0ºC under atmospheric conditions (1013.3 hPa).		Y	1	Smeykal, H (2005), Transfluthrin (Bayothrin), NAK 4455: Flash Point , Siemens AG, Prozess-Sicherheit Report No. 20050216.02 BES Ref: M-254399-01-1 30.05.05 GLP. Unpublished	X
3.13 Surface tension (IIA3.10)			44.8 ± 3.0 dyne/cm [predicted using Chemsketch 5.0 (Advanced Chemistry Development Inc)**]**	Due to limited exposure to aquatic environmental compartments and the availability of a model-predicted value, the need to conduct a study on the surface tension of transfluthrin active substance is considered to be scientifically unjustified			A detailed waiver has been provided (see justification for non – submission of data Section 3.13)	

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Section A3 Physical and Chemical Properties of Active Substance								
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.14 Viscosity (-)	Based on EPA OPPTS 830.7100, DIN 51562 and OECG guideline 114	Batch No. EATFTJ005, 99.1% (w/w)	181.9 mPa·s at 20ºC 35.65 mPa·s at 40ºC		Y	1	Rexer, K and Bittner, P (2005) Physical, Chemical and Technical Properties of Transfluthrin, Bayer CropScience GmbH, Report No. WIR0132 (PC) 01 BES Ref: M-253445-01-1 02.06.05 GLP, unpublished	X
3.15 Explosive properties (IIA3.11)	Investigated as stipulated in test EC A14 and OECD guideline 113	Batch No. EATFTJ005, 99.1% (w/w)	Non-explosive according to mechanical sensitivity (shock and friction) and thermal sensitivity tests	Mechanical (friction): No explosion using a pinload with 360 N.; (shock): no explosion using 10 kg mass falling from 0.4 m ht.; Thermal: no explosion within 3 tests using circular nozzle with hole 2 mm diameter.	Y	1	Smeykal, H (2005) Transfluthrin (Bayothrin), NAK 4455: Explosive Properties A.14., Siemens AG Prozess-Sicherheit, Report No. 20050216.03 BES Ref: M-251690-01-1 30.05.05 GLP. unpublished	X

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Section A3	Physical and Chemical Properties of Active Substance							
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.16 Oxidizing properties (IIA3.12)	Investigated as stipulated in EC test procedure A21 for the oxidising properties of liquids.	Batch No. EATFTJ005, 99.1% (w/w)	Non-oxidising according to tests conducted under EC A21. Transfluthrin does not have oxidising potential.	The 1:1 mixture, by mass, of test item and cellulose has a mean pressure rise time higher than that of a 1:1 mixture of 65% nitric acid and cellulose and did not reach the bursting pressure of the rupture disc. Result is confirmed by the *absence* of moieties in the molecular structure which are know to confer oxidising properties.	Y	1	Smeykal, H (2006) Transfluthrin (Bayothrin), NAK 4455; Substance, technical AE 0035474 00 1D99 0004. Oxidizing properties of liquids A.21., Siemens AG Prozess-Sicherheit, Report No. 20050216.03 BES Ref: M-268646-01-1 29.03.06 GLP. unpublished	X
3.17 Reactivity towards container material (IIA3.13)	Stability in metal containers stored at ambient and 40°C, 75% r.h. for period of 6 months was investigated following in-house procedures.	Technical grade Transfluthrin, Batch No. 921216ELB01, Purity: 95.3%	Transfluthrin did not decompose when stored in metal containers for up to 6 months at either ambient temperature or at 40°C, 75% r.h.	Three lots tested showed minimal or no change in appearance, content of active ingredient, known impurities, water, acidity and alkalinity.	Y	1	Diehl, H (1998), Final Stability Report, NAK 4455 Techn., A & M Stabtest, Bayer AG, Study No. ST 033/97. BES Ref: M0-03-010451 GLP, Unpublished	X

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-03-2007
Evaluation of applicant's justification	*3.1.1. Melting point:* a) AE 003547 00 in reference should be changed to AE 0035474 00. b) "Pont" in reference should be changed to "point".
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-03-2007
Evaluation of applicant's justification	*3.1.3 Bulk density:* a) According to the study report, the reported values are relative densities. Relative density is dimensionless and therefore has no unit (-).
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-03-2007
Evaluation of applicant's justification	*3.2 Vapour pressure:* a) BES reference (MO-04-003000) should be added to reference. b) Vapour pressure was measured between 28 and 82 °C. c) It was not possible to measure the vapour pressure at ambient temperature directly, because the pressures were too low. d) Vapour pressure was extrapolated from measurements between 28 and 82 °C. However, the melting point of 32 °C lies within this temperature interval. The reported vapour pressures of $9x10^{-4}$ Pa (20°C) and $2x10^{-3}$ Pa (25 °C) is questionable as extrapolation through a phase change is usually unreliable. However, the vapour pressure curve suggests that the melting of the substance does not significantly influence results as the curve remains straight. Endpoint: $9x10^{-4}$ Pa at 20 °C.
Conclusion	Acceptable.
Remarks	Reliability is 2.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-03-2007
Evaluation of applicant's justification	*3.3 Henry's Law Constant:* The applicant claims GLP, but this is considered a minor issue. The Henry's Law Constant was calculated and not experimentally determined.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	

Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.4 Absorption spectra (UV/VIS):* a) Molar extinction (ε) was calculated by RMS (based on A = ε x d x c). A ($mol^{-1}cm^{-1}$) @ 277.5nm = 0 -> ε = 0 L/mol.cm A ($mol^{-1}cm^{-1}$) @ 270.0nm = 0.05 -> ε = 130 L/mol.cm A ($mol^{-1}cm^{-1}$) @ 250.0nm = 0.01 -> ε = 26 L/mol.cm A ($mol^{-1}cm^{-1}$) @ 210.0nm = 0.70 -> ε = 1819 L/mol.cm No absorption observed above 290 nm
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2006

Evaluation of applicant's justification

3.4 Absorption Spectra (IR):

Reported absorbance:

absorbance (cm^{-1})	signal
3426	weak
3080-3072	weak
3047	weak
3003	weak
2988-2928	weak
1737-1720	middle
1697	weak
1620	weak
1506	strong
1462	weak
1446	weak
1426	weak
1391-1378	weak
1346	weak
1302	weak
1277	weak
1265	middle
1224	middle
1177-1141	middle - strong
1112	middle
1089	weak
1060	weak
1048	weak
1028	weak
1017	weak
992	weak
983	weak
966	weak
941	weak
931	weak
915-879	weak – middle
866-854	middle
822	weak
764	weak
747	weak

713	weak
667	weak
646	weak
629	weak
548	weak
527	weak

3.4 Absorption Spectra (NMR):

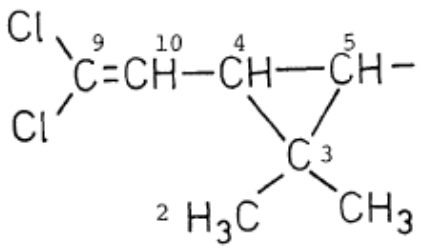
Tetramethylsilan (TMS) was used as internal standard.

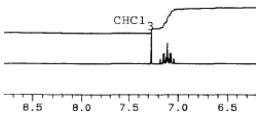
Reported peaks and multiplicity for H- and C-atoms:

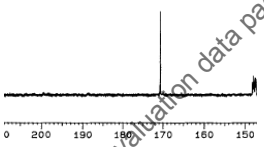
H-atom peaks (ppm)	Multiplicity	C-atom peaks	Multiplicity
1.29	singlet	20.03	quadruplet
1.19	singlet	22.53	quadruplet
2.27	doublet	29.41	singlet
1.61	doublet	33.24	doublet
5.25	multiplet	34.35	doublet
7.10	multiplet	53.88	triplet
5.60	doublet	106.79	doublet
		115.27	singlet
		122.45	singlet
		126.70	doublet
		145.25	singlet
		145.81	singlet
		170.48	singlet

NMR spectra as included in the report (^{1}H-NMR and ^{13}C-NMR spectra):

Structure:







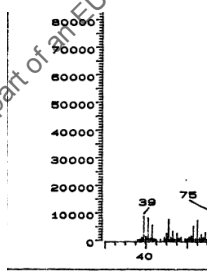
Hydrogen-atom	Chemical shift	Multiplicity	Relative no. of atoms

H-Atome (a)	Chem. Verschieb. (ppm)
H-1 oder H-2	1,29
H-2 oder H-1	1,19
H-4	2,27
H-5	1,61
H-6	5,25
H-7	7,10
H-10	5,60

a) Strukturformel Seite 8

b) S = Singulett
D = Dublett
M = Multiplett

Carbon-atom	Chemical shift	Multiplicity	Relative no. of atoms

	C-11 oder C-12 145,25 C-12 oder C-11 145,81 C-13 170,48 --- a) Strukturformel Seite 8 b) S = Singulett D = Dublett T = Triplett Q = Quadruplett
	3.4 Absorption Spectra (MS): Peaks were observed at 370 (M), 335 (M+ - Cl), 191 (M+ - O-CH_2-C_6HF_4), 163 (m/z 191 – CO), 143 (m/z 163 – HF), 127 (m/z 163 – HCl) and 91 (m/z 127 – HCl) m/z
	
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.5 Solubility in water:* a) The reported confidence interval of 2.94 should be 0.00294. b) No information on the validation of the method of analysis is provided. LOD and LOQ are missing. The study report does not contain a chromatogram and it is unclear which substance is used as external standard (NAK4455?). However, since the column-elution method (OECD Guideline 105) is sufficiently standardised, the resulting water solubility is considered acceptable
Conclusion	acceptable.
Remarks	-
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.6 Dissociation constant:* Change under method: “Titration, spectrophotometric, and conductometric methods in accordance with OECD Guideline 112” to “Statement on Titration, spectrophotometric, and conductometric methods in accordance with OECD Guideline 112”.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	

Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)* Reported values are considered to be unrealistically high (e.g. 10-20 kg/L in acetone). Transfluthrin is considered to be completely miscible in any ratio in the tested organic solvents.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.9 Partition coefficient n-octanol/water:* a) Shake flask method can be used to determine log Kow values between -2 and 4 (occasionally up to 5). For higher log Kow values, OECD Guideline 117 (using HPLC) or Draft Guideline 123 (slow-stirring method) is advised. The value of 5.46 is not considered acceptable. b) No information on the validation of the method of analysis is provided (e.g. LOQ, LOD, a representative chromatogram, identity of external standard is unclear (NAK 4455?)). Estimation with Bioloom yields a calculated log K_{ow} of 5.94, EPIWIN v3.2 yields a value of 6.17.
Conclusion	Acceptable – study not required for risk assessment.
Remarks	A log Pow is not required as an accepted BCF fish is available (please refer to the environmental section for details). Epiwin calculations are considered acceptable. Furthermore, a Koc value is available.

	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.10 Thermal stability:* Addition to reference: AE 0035474 00 1D99 0004 (see also reference for 3.1.1 Melting point).
Conclusion	Acceptable.
Remarks	None
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.12 Flash point:* In another reference (Heitkamp, 2001, MO-03-010048, corresponding to endpoint 3.11: auto-ignition temperature), a flash point of 122 °C was determined according to EC Guideline A9.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*

Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	23-04-2007
Evaluation of applicant's justification	*3.13 Surface tension:* If water solubility is < 1 mg/L, surface tension does not need to be tested.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.14 Viscosity:* a) Under 'Method', OECG should be OECD (typing error). b) Measuring viscosity at 20 °C is not required and considered invalid, since the substance is a solid at this temperature (melting point 32 °C). c) The viscosity at 40 °C is considered acceptable.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	

Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.15 Explosive properties:* According to the study report, after the mechanical sensitivity tests (shock), the colour of the substance changed to light brown due to decomposition of the test item.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.15 Oxidising properties:* a) The test method for the oxidising properties of liquids and not the test method for solids was used, due to the fact that the test item melts already at a temperature of 32 °C and therefore it was not possible to grind the test item to a particle size < 125 µm. b) In two instances the bursting pressure of the rupture disc (2200 kPa) was reached.
Conclusion	Acceptable.
Remarks	None.

	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Evaluation by Competent Authorities

	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-03-2007
Evaluation of applicant's justification	*3.17 Reactivity towards container material:* a) In lot no. 816 779 003 one impurity was found in concentrations of about 0.1% , both at the start and end of the experiment. b) Metal container specification: Material: Black metal (standard steel sheet to EN 0130-DC 01-AM) with inner coating. Volume: 6L Weight (empty): 1.3 kg Diameter: 230 mm Height: 178 mm Wall thickness: 0.5 mm Coating inside: A 7 lacquer Furthermore, according to the applicant, the technical grade active substance is only transported to formulation plants in the original containers used for shipment. There is no intermediate transfer of the technical material to other containers before it arrives in the formulation factories for production into end-use formulated products.
Conclusion	Acceptable.
Remarks	None.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

Doc IIIA/ Section 3.13 **BPD Data Set IIA/ Annex Point III.3.10**	**Surface tension**	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ]	**Technically not feasible [ ]** **Scientifically unjustified [✓]**	
Limited exposure [✓]	**Other justification [ ]**	
Detailed justification:	Transfluthrin is a colourless to off-white crystalline solid with needle-like appearance. It has a very low solubility in water (0.057 ± 2.94 mg/L, at 20˚C). Its viscosity, according to OECD 114, is 181.9 mPa/s at 20ºC. The surface tension test method measures the reduction of surface tension of water by dissolving the substance in it. Surface tension data are relevant for the environment as surface active compounds can affect wettability of membranes, act as emulsifiers and affect interfacial properties between environmental compartments influencing degradation processes. Accordingly, Chemsketch 5.0 has been used to predict a surface tension value for transfluthrin of = 44.8 ± 3.0 dyne/cm.[Chemsketch 5.0 is a product developed by Advanced Chemistry Development Inc., for the prediction of simple, chemical properties for molecules see www.acdlabs.com]. The formulated products, fan-assisted vaporiser, and anti-moth disc, are for indoor use only. During use of these and the formulated mosquito coil product, the active substance is volatilised. Environmental exposure from these uses of transfluthrin is predicted to be minimal (refer to document II-B, section 3.3). In addition, due to the high lipophilic property of transfluthrin (log Pow 5.46) and low water solubility, the limited amounts of compound predicted in sewage water are unlikely to even reach the environment through wastewater. Due to limited exposure to aquatic environmental compartments and the availability of a model-predicted value, the need to conduct a study on the surface tension of transfluthrin active substance is considered to be scientifically unjustified.	X
Undertaking of intended data submission [ ]	Not applicable	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	22-02-2007
Evaluation of applicant's justification	Applicant's justification is considered to be acceptable. It has to be noted though that for substances with a water solubility of < 1 mg/L surface tension does not need to be tested.
Conclusion	Acceptable.
Remarks	Recalculation of the surface tension using ChemSketch 8 yielded a similar value as reported by the applicant.
	COMMENTS FROM OTHER MEMBER STATE *(specify)*
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	