Section	on A3	Physical and Cher	nical Properti	es of Active Substance					
Subse (Anne	ction ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.1	Melting point, boiling point, relative density (IIA3.1)								
3.1.1	Melting point	EC method A.1 (92/69/EEC) OECD guideline 102 Differential scanning calorimetry (DSC) and capillary method	Specification as given in Section A2	The substance has no melting point at atmospheric pressure (1013.3 hPa); decomposition occurs before melting at approx. 205 °C (also see A3.10 below).		Υ		A3.1.1/01:  Potassium sorbate powder – Melting point/ melting range, boiling point/ boiling range, vapour pressure.	
3.1.2	Boiling point	EC method A.2 (92/69/EEC) OECD guideline 103 Differential scanning calorimetry (DSC)	Specification as given in Section A2	The substance has no boiling point at atmospheric pressure (1013.3 hPa); decomposition occurs before boiling		Υ	<b>1</b> 1,	Cross-reference: A3.1.1/01	

Secti	on A3	Physical and Cher	nical Propertio	es of Active Substance					_
	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.1.3	Bulk density/ relative density	EC method A.3 (92/69/EEC) OECD guideline 109 Air comparison pycnometer	Specification as given in Section A2	DR <sub>4</sub> = 1.36 Test temperature = 23.5 °C		Y	1	A3.1.3/01; Potassium sorbate powder — Relative density.	
3.2	Vapour pressure (IIA3.2)	EC method A.4 (92/69/EEC)  OECD guideline 104  Effusion method: Vapour pressure balance  The substance was additionally degassed at 50 ± 5 °C under a vacuum of 10-5 hPa for 16 hours.	Specification as given in Section A2	The vapour pressure remained below the detection limit of $10^{-5}$ hPa in the temperature range between 25 an 148 °C.  The following conservative estimates are reported:  p $(20  ^{\circ}\text{C}) \le 1.0 \times 10^{-7}$ hPa p $(25  ^{\circ}\text{C}) \le 1.0 \times 10^{-7}$ hPa p $(50  ^{\circ}\text{C}) \le 1.0 \times 10^{-7}$ hPa		Y	1	Cross-reference: A3.1.1/01	

				Dossier amendment February 2009 Page 3 of 26					
Sectio	on A3	Physical and Cher	nical Propertie	s of Active Substance					
Subsec	ction x point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.2.1	Henry's Law Constant	a) Calculation based on measured vapour pressure and water solubility b) QSAR estimate using program Henrywin	Not applicable (calculation)	a) experimentally based:  H = 2.77 × 10 <sup>-9</sup> Pa × m <sup>3</sup> /mol  b) QSAR estimates:  H = 5.72 × 10 <sup>-5</sup> Pa × m <sup>3</sup> /mol  (bond contributions)  H = 4.99 × 10 <sup>-6</sup> Pa × m <sup>3</sup> /mol  (group contributions)	The estimate based on experimental data is considered to be more reliable since the QSAR model is unable to take into account the ionic nature of the test substance in solution.	n.a.		A3.2.1/01:  Mode calculation of Henry's constant of Potassium sorbate.	law A
	Appearance (IIA3.3)								
3.3.1	Physical state	Visual inspection	Specification as given in Section A2	Solid Crystalline powder		Υ	1	Cross-reference; A3.1.1/01:	

Section	n A3	Physical and Cher	nical Properti	es of Active Subs	tance				
Subsec (Annex	tion point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Offici use only
3.3.2	Colour	Visual inspection	Specification as given in Section A2	White		Y	τ	Cross-reference: A3.1.1/01	
3.3.3	Odour	Olfactory assessment	Specification as given in Section A2 no specific batch tested	Odourless		N	<b>T</b>	Cross-reference: Material safety data sh	eel

			724	Potassiu	ım sorbate			Dossier amendment Febru Pag	ary 2009 e 5 of 26
Secti	on A3	Physical and Cher	nical Properti	es of Active Substance					
	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.4	Absorption spectra (IIA3.4)								
	UV/VIS	OECD 101	Specification as given in Section A2			Y	1	A3.4.1/01:  Determination of the UV-VIS spectrum of Potassium sorbate.	
	IR (Sorbic acid)	Guideline: not applicable Method: Infrared spectroscopy	Specification: Sorbic acid	A graphical presentation of the IR spectrum is given in Figure A3- 4. The spectrum is considered to be in accordance with the proposed structure of the test substance.	This IR spectrum was recorded for Sorbic acid. Since the Sorbate anion is the determinant of the spectral properties of Sorbic acid as well as of Potassium sorbate, the submitted spectrum is also considered to be representative for Potassium sorbate. However, for the sake of completeness a non-GLP spectrum of Potassium sorbate from a public source is also provided below.	Y	1	Determination of the IR spectrum of Sorbic acid.	

Section A3	Physical and Cher	nical Propertie	es of Active Substance					1
Subsection (Annex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
IR (Potassium sorbate)	Guideline: not applicable Method; Infrared spectroscopy. KBr disc	Specification: not stated Batch no.: not stated Expiry date: not stated Purity: not stated	A graphical presentation of the IR spectrum is given in Figure A3-5.		N	0 (Reliability not assignable due lack of documentation)	A3.4.2/02: Anonymous (2004) IR spectrum (KBr disc). Potassium sorbate. http://www.aist.go.jp/ RIODB/SDBS/sdbs/owa/ sdbs_sea.cre_frame_disp? sdbsno=752 (accessed June 25, 2004).	
†H-NMR (1)	Guideline: not applicable Method: <sup>1</sup> H-NMR spectroscopy	Specification: Sorbic acid	A graphical presentation of the <sup>1</sup> H-NMR spectrum is given in Figure A3-6.  The spectrum is considered to be in accordance with the proposed structure of the test substance.	The <sup>1</sup> H-NMR spectrum was recorded for Sorbic acid. A corresponding spectrum for Potassium sorbate will be submitted in due course, as also stated in a separate justification form.	Y	1	A3.4.3/01:  Determination of the <sup>1</sup> H- NMR specirum of Sorbic acid.	
H-NMR (2)	Guideline: not applicable Method: <sup>1</sup> H-NMR spectroscopy	Specification as given in Section A2	A graphical presentation of the <sup>1</sup> H-NMR spectrum is given in Figure A3-7.  The spectrum is considered to be in accordance with the proposed structure of the test substance.		N	2	Potassium sorbate. lot # 9972, identification with NMR spectroscopy.	

Section A3	Physical and Cher	nical Propertie	es of Active Substance					
Subsection (Annex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Offici use only
<sup>13</sup> C-NMR	Guideline: not applicable Method: <sup>13</sup> C-NMR spectroscopy	Specification: Sorbic acid	A graphical presentation of the <sup>13</sup> C-NMR spectrum is given in Figure A3- 8.  The spectrum is considered to be in accordance with the proposed structure of the test substance.	The <sup>13</sup> C-NMR spectrum was recorded for Sorbic acid. Since the Sorbate anion is the determinant of the spectral properties of Sorbic acid as well as of Potassium sorbate, the submitted spectrum is also considered to be representative for Potassium sorbate.	Y	1:	Determination of the <sup>13</sup> C-NMR spectrum of Sorbic acid.	
MS	Guideline: not applicable Method: high resolution mass spectroscopy	Specification: Sorbic acid	A graphical presentation of the mass spectrum is given in Figure A3-9.  The spectrum is considered to be in accordance with the proposed structure of the test substance.	The mass spectrum was recorded for Sorbic acid. Since the Sorbate anion is the determinant of the spectral properties of Sorbic acid as well as of Potassium sorbate, the submitted spectrum is also considered to be representative for Potassium sorbate.	Υ	1	Determination of the GC/MS analysis of Sorbic acid.	

				Potassium	n sorbate			Dossier amendment Febru Pag	ary 2005 e 8 of 26
Secti	ion A3	Physical and Cher	nical Properti	es of Active Substance					
	ection ex point)	Metbod/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.5	Solubility in water (IIA3.5)	EC method A.6 (92/69/EC) OECD guideline 105 Flask method Concentrations of the test substance were determined by HPLC analysis; linearity of detector response is ensured (R > 0.999).	Specification as given in Section A2	The solubility varied in a range between 1.5 and 563 g/l, depending on pH and temperature. More details are given in Table A3-1.  The solubility at pH 4 and 7 had to be extrapolated because an experimental determination was impossible due to the depletion of buffer capacity by the saturated solution of Potassium sorbate.		Y	1	A3.5/01:  Water solubility of Potassium sorbate.	
3.6	Dissociation constant (-)	OECD 112 Spectrophotometric method	Specification as given in Section A2	$pK_a = 4.69 \pm 0.03 \text{ (SD)}$		Y	1	A3.6/01:  Dissociation constant of Potassium sorbate.  Arbeitsgemeinschaft	1

Sect	ion A3	Physical and Chen	nical Propertie	es of Active Substance			-	-	
	section nex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.7	Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Adapted EC A.6 and OECD 105, flask method	Specification as given in Section A2	Methanol:  10 °C: 79.4 ± 0.3 mg/l  20 °C: 79.0 ± 0.8 mg/l  30 °C: 79.3 ± 0.8 mg/l  p-Xylene:  10 °C: 30.3 ± 0.1 mg/l  20 °C: 30.5 ± 0.1 mg/l  The solubility of  Potassium sorbate in organic solvents was essentially independent of temperature.		Y	1	A3.7/01:  Solubility of Potassium sorbate in two organic solvents.	
3.8	Solubility in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)				Data not considered to be required, since the biocidal product is an aqueous solution containing no further (organic) solvents.				
3.9	Partition coefficient n- octanol/water (IIA3.6)	EC method A.8 - HPLC method - Linearity of analytical system ensured: $r^2$ (pH 2.5) = 0.981: $r^2$ (pH 6.5) = 0.980 for log $P_{one}$ vs. log $k$	99.9 % Sorbic acid (by titration)	$log P_{ov}$ (pH = 2.5) = 1.32 $log P_{ov}$ (pH = 6.5) = -1.72 Temperature: 20 ± 2 °C	Extrapolation from Sorbic acid is not considered to be restricted in any way since the Sorbate anion is the moiety of interest and the ratio of free acid vs. dissociated anion entirely depends on pH.	Y	Ì	A3.9/01:  Partition coefficient of Sorbic acid (HPLC method).	

				Potassiur	n sorbate			Dossier amendment Februarien Page	ary 2005 10 of 26
Sect	on A3	Physical and Cher	nical Properti	es of Active Substance					
	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.10	Thermal stability, identity of relevant breakdown products (IIA3.7)	OECD 113 Differential scanning calorimetry	Specification as given in Section A2	An endothermic effect (transformation process) was observed in the temperature range 150–175 °C, and an exothermal effect in the temperature range 205–320 °C.		Y	1	Cross-reference: A3.1.1/01	
3.11	Flammability, including auto- flammability and identity of combustion products (11A3.8)	Flammability: EC method A.10 Auto-flammability: EC method A.16	Specification as given in Section A2	Not highly flammable Self-ignition temperature: 178 °C		Y	1	Potassium sorbate – Flammability (solids) and auto-flammability (solids – determination of relative self-ignition temperature).	

Physical and Cher	nical Properti	es of Active Substan	ce					
Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference		Officia use only
			Experimental data are not submitted since these are considered to be scientifically unjustified:	-			>	X
			From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file.					
			Experimental data are not submitted since these are considered to be				X	X
			From the structural formula and the composition of the substance it can be safely concluded that the substance is stable in air at room temperature and is not pryophoric.					
		Method/Guideline Purity/	Method/Guideline Purity/ Results	Method/ Guideline Purity/ Specification  Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file. Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance is stable in air at room temperature and is not pryophoric.	Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file.  Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance is stable in air at room temperature and is	Method/Guideline Purity/ Specification Results Remarks/Justification GLP (Y/N)  Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file.  Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance is stable in air at room temperature and is not pryophoric.	Method/ Guideline Purity/ Specification Results Remarks/Justification GLP (Y/N) Reference (Y/N)  Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file. Experimental data are not submitted since these are considered to be scientifically unjustified: From the structural formula and the composition of the substance it can be safely concluded that the substance it can be safely concluded that the substance is stable in air at room temperature and is not pryophoric.	Method/ Guideline Purity/ Specification Results Remarks/Justification GLP (Y/N) Reference Purity/ Specification Results Remarks/Justification GLP (Y/N) Reference Respectively.  Experimental data are not submitted since these are considered to be scientifically unjustified:  From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.  This justification is also given in a separate file.  Experimental data are not submitted since these are considered to be scientifically unjustified:  From the structural formula and the composition of the substance it can be safely concluded that the substance is stable in air at room temperature and is not pryophoric.

				Potassiu	m sorbate	70.5		Dossier ame	endment Februa Page	ary 2005 12 of 26
Secti	on A3	Physical and Cher	nical Properti	es of Active Substance					_	
Subse (Ann	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference		Official use only
3.12	Flash-point (IIA3.9)				Not applicable.  A test on this endpoint must be provided for liquids whose vapours can be ignited; this does not apply to Potassium sorbate, which is a solid with low vapour pressure.					X
3.13	Surface tension (IIA3,10)	EC method A.5, OECD 115	Specification as given in Section A2	σ = 72.6 mN/m at 20°C Potassium sorbate is therefore not a surface active substance.	Test conc. = 1 g/l	Y	1	tension of Posorbate. Rep 20031475/0	ort No.	
3.14	Viscosity (-)				Not applicable.  Data are not considered to be required since the active substance is solid.					X

			Potassium sorbate				Dossier amendment February 2005 Page 13 of 26		
Secti	on A3	Physical and Chemical Properties of Active Substance							
Subse (Anne	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Officia use only
3.15	Explosive properties (IIA3.11)	Model calculation (software model CHETAH 7.2)	Model calculation conducted for Sorbic acid, but extrapolation to Potassium sorbate is not considered to be restricted in any way.	Maximum heat of decomposition = -479 cal/g  Difference between heat of combustion and heat of decomposition = -5904 cal/g  Oxygen balance = -200 %  In conclusion, structural aspects and estimated thermodynamic properties indicated that Sorbic acid lacks explosive properties.	In EC method A.14, it is expressly mentioned that an experimental determination of the explosivity of a compound is not required, if available thermodynamic data (reaction enthalpies) and/or the absence of certain reactive groups in the structural formula indicate that the substance will not decompose violently under formation of gases or release of energy (and thus does not pose a risk for explosivity). Thus, the conduct of further experimental verification is not considered to be required.	n.a.	1	A3.15/01:  Explosivity of Sorbic acid technical.	X

				Potassiur	m sorbate			Dossier amendment F	ebruary 2005 Page 14 of 26
Secti	on A3	Physical and Cher	nical Propertie	es of Active Substance					31
Subse (Ann	ection ex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.16	Oxidizing properties (IIA3.12)	Model calculation (software model CHETAH 7.2)	Model calculation conducted for Sorbic acid, but extrapolation to Potassium sorbate is not considered to be restricted in any way.	Maximum heat of decomposition = -479 cal/g  Difference between heat of combustion and heat of decomposition = -5904 cal/g  Oxygen balance = -200 %  In conclusion, structural aspects and estimated thermodynamic properties indicate that Sorbic acid is more of a combustible nature, than considered to possess oxidising properties.	In EC method A.17, it is expressly mentioned that an experimental determination of the oxidising properties of a compound is not required if available thermodynamic data and the absence of certain reactive groups in the structural formula indicate that the substance will not react exothermally with combustible material. Thus, the conduct of further experimental verification is not considered to be required.	n. a.	1	A3.16/01:  Oxidising properties of Sorbic acid technical.	X
3.17	Reactivity towards container material (IIA3.13)				Polyethylene has been used as lining material for potassium sorbate for decades. Polyethylene is inert to potassium sorbate and vice versa.				

**Evaluation by Competent Authorities** 

			P	otassium sorbate	Hr	Dossier amendmer	nt February 200 Page 15 of 2
Section A3	Physical and Chem	ucal Properti	es of Active Sub	stance			
Subsection (Annex point)	Method/ Guideline	Purity/ Specification	Results	Remarks/Justification	GLP Reliability (Y/N)	Reference	Offici use only
	Use separate " to the commer	evaluation be ats and views	oxes" to provide s submitted	transparency as			
	EVALUA	ATION BY R	APPORTEUR	MEMBER STATE			
Date							
3.2.1				<del></del>		i	
	15						
3.11, ECC A12, ECC	A13;						
3.12, ECC A9;							
3.14							
3.15							
3.16	-						
Reliability	<u> </u>						
Acceptability							
	COMME	NTS FROM					
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	Potassium sorbate	Dossier amendment February 2005 Page 16 of 26					
Section A3	Physical and Chemical Properties of Active Substance						
Subsection (Annex point)	Method/Guideline Purity/ Results Remarks/Justification GI (Y	[Hanner					
Date	Give date of comments submitted						
	Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary conclusion.  Discuss if deviating from view of rapporteur member state						
	Discuss if deviating from view of rapporteur member state						
Reliability	Discuss if deviating from view of rapporteur member state						
Acceptability	Discuss if deviating from view of rapporteur member state						
Remarks							

Table A3- 1: Solubility of Potassium sorbate in water at different pH values and temperatures.

Temperature [°C]	Solubility [g/l]			
	4 (1)	рН 7 <sup>(2)</sup>	9 (3)	
10	1.50	539	539	
20	1.95	543	543	
30	2.85	563	563	

<sup>(1)</sup> calculated from water solubility of Sorbic acid under titration with sodium base

<sup>(2)</sup> extrapolated from experimentally determined values at pH = 9

<sup>(3)</sup> experimentally determined average values

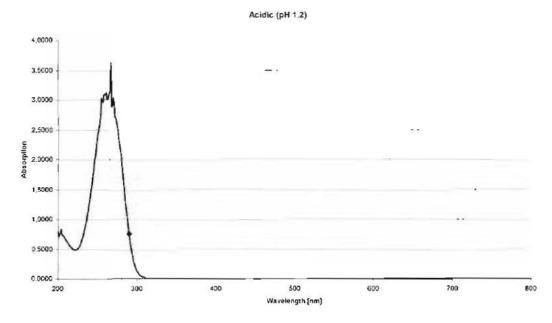


Figure A3-1: UV/VIS spectrum of Potassium sorbate at pH 1.2.

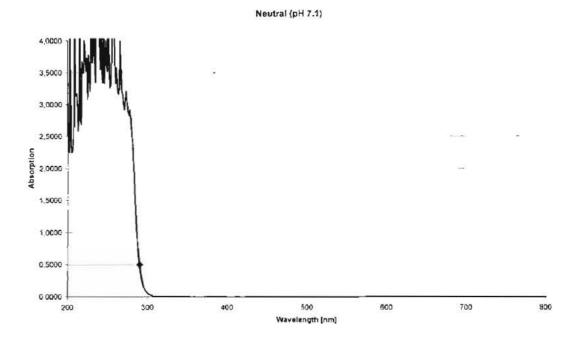


Figure A3-2: UV/VIS spectrum of Potassium sorbate at pH 7.1.

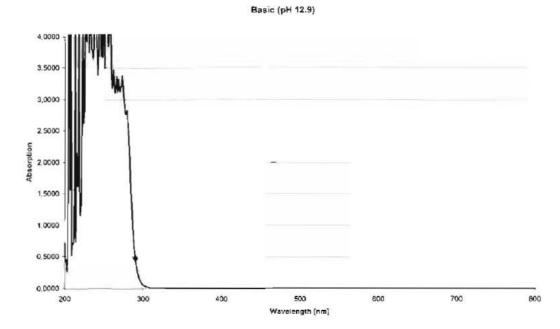


Figure A3- 3: UV/VIS spectrum of Potassium sorbate at pH 12.9.

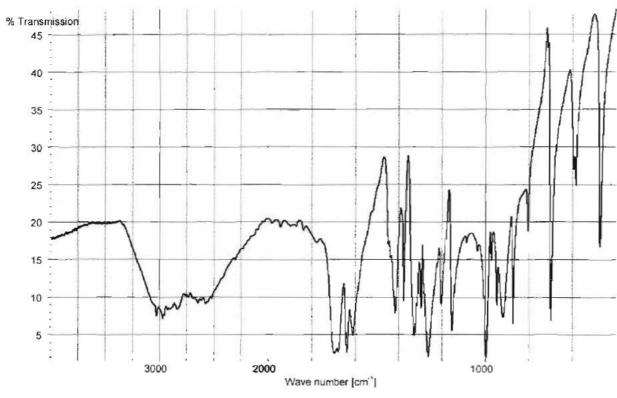


Figure A3- 4: IR spectrum of Sorbic acid.

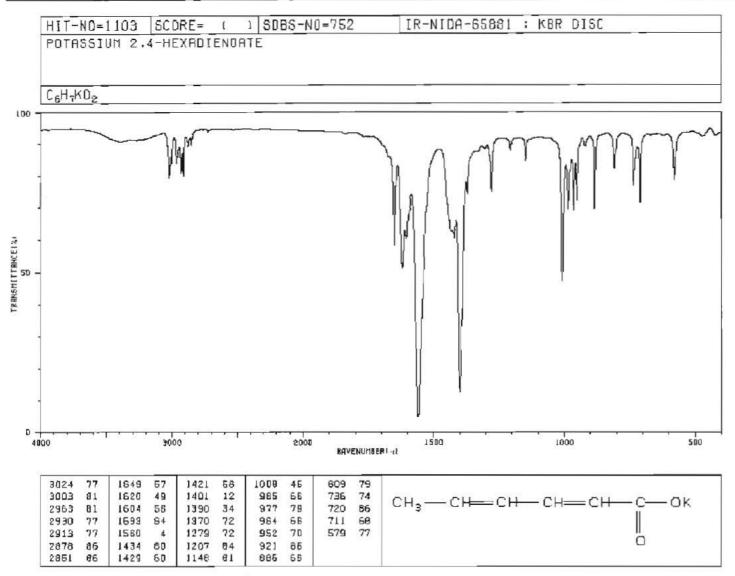


Figure A3- 5: IR spectrum of Potassium sorbate.

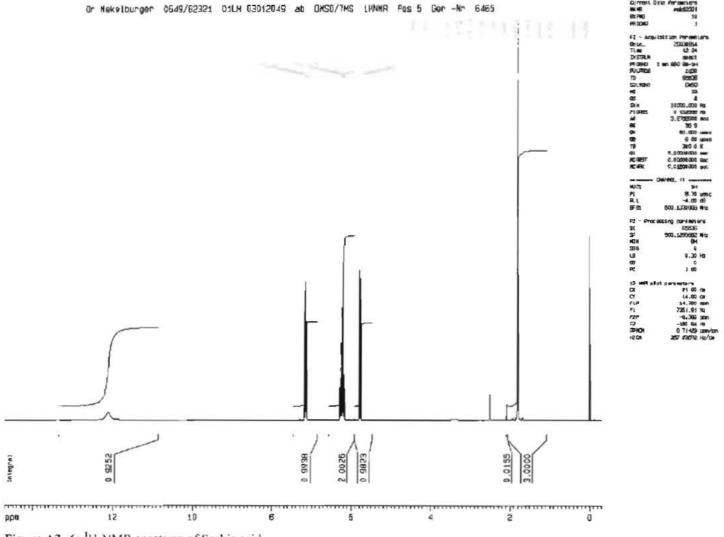


Figure A3- 6: <sup>1</sup>H-NMR spectrum of Sorbic acid.

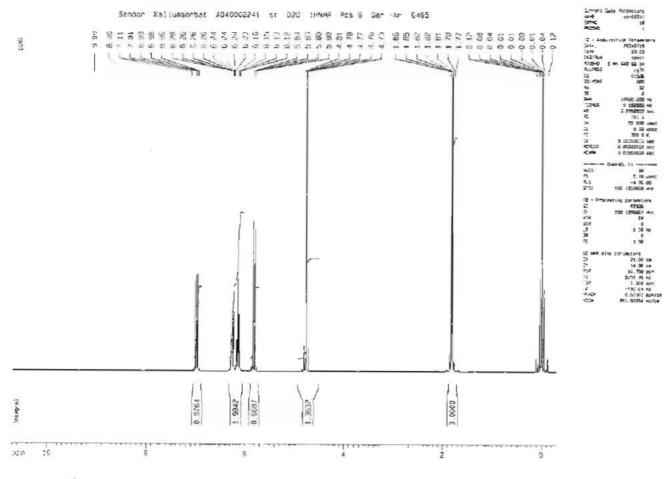


Figure A3- 7: H-NMR spectrum of Potassium sorbate.

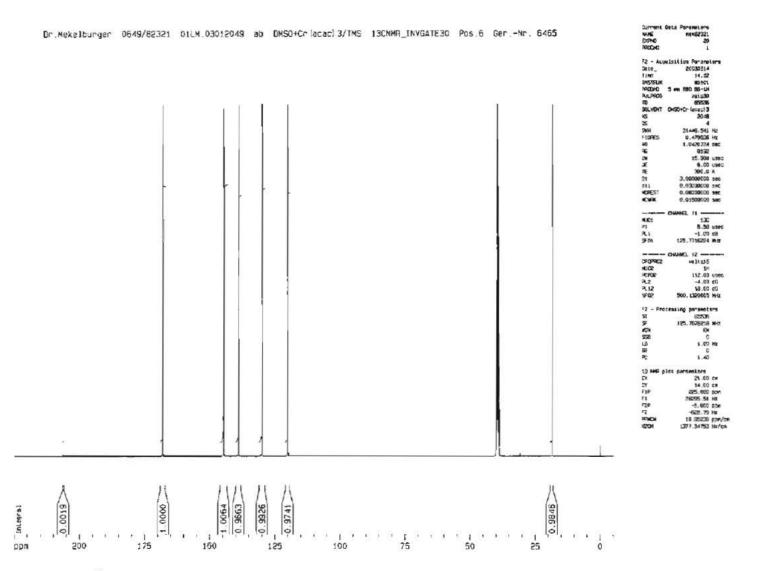


Figure A3-8: <sup>13</sup>C-NMR spectrum of Sorbic acid.

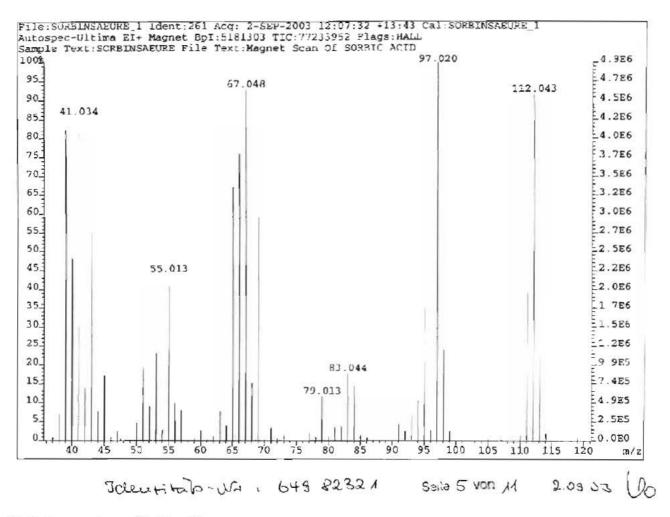


Figure A3-9: Mass spectrum of Sorbic acid.

Section A3.4
Annex Point IIA3.4

## Absorption spectra

Official use only

## JUSTIFICATION FOR NON-SUBMISSION OF DATA

Other existing data |X|

Technically not feasible [X]

Other justification | 1

Scientifically unjustified |X|

Detailed justification:

Limited exposure

IR, <sup>13</sup>C-NMR and MS spectra were submitted for Sorbic acid instead of Potassium sorbate, with the following justification:

General justification for IR, 13C-NMR and MS:

- (i) In the environment as well as in biological media, the Sorbate anion is the active principle, which can not adequately be characterised spectroscopically for obvious reasons, which is why it is felt that the spectral characterisation of Sorbic acid should be sufficient.
- (ii) Further, since the "Sorbate moiety" is the sole determinant of the spectral properties of both Sorbic acid and of Potassium sorbate, the submitted spectra on Sorbic acid are considered to be also representative for Potassium sorbate. Substitution of the proton of Sorbic acid by a Potassium cation is not feasibly expected to alter the spectral properties regarding IR and <sup>13</sup>C-NMR to any relevant extent. However, concerning the <sup>1</sup>H-NMR spectrum, differences between Potassium sorbate and Sorbic acid are inevitably to be expected due to the replacement of protons by potassium cations, which is why this type of data is provided in the current dossier amendment.
- (iii) Regarding the characterisation of the active substance (purity, impurities), the determination of specific spectra (IR, <sup>13</sup>C-NMR) is considered to be irrelevant: Both substances are produced according to specifications of EU food law (Directive 96/77/EC), fulfilling an active ingredient content of > 99 % (w/w). The impurity profile is nearly identical for both Sorbic acid and Potassium sorbate. The only relevant additional impurity of Potassium sorbate is Sorbic acid itself, since Potassium sorbate is manufactured from food-grade Sorbic acid by neutralisation with Potassium hydroxide (see Section 2 of this dossier). Thus, any impurities of concern are obviously not to be expected.

Specific additional justifications regarding particular spectra:

IR: The standard method for sample preparation for recording an IR spectrum is powdering the test substance with Potassium bromide. This method was also followed in the case of Sorbic acid (see A3.4.2/01). In view of this technical peculiarity, the determination of a specific IR spectrum for Potassium sorbate is not considered to be feasible since the presence of Potassium in the KBr spectral matrix will obviously overlay any Potassium that is introduced additionally through replacing Sorbic acid by Potassium sorbate. It may therefore be expected that the two spectra would be indistinguishable. Thus, no further gain of information is expected from the GLP-compliant recording of an IR spectrum for Potassium sorbate. An IR-spectrum of Potassium sorbate from a public source is nevertheless provided in the dossier.

NMR: A <sup>1</sup>H-NMR spectrum is provided in section A3 of the current dossier amendment. With regard to the <sup>13</sup>C-NMR spectrum, however, the spectral properties are solely determined by the Sorbate anion in any case, since only influenced by the arrangement of the C-atoms. Consequently, Potassium sorbate and Sorbic acid will be indistinguishable due to the structural identity of the spectroscopically relevant moiety. Thus, no further gain of information is expected from

## Absorption spectra

the recording of a <sup>13</sup>C-NMR spectrum for Potassium sorbate.

MS: The determination of a mass spectrum requires vapourisation and ionisation of the test substance. The absence of a boiling point and a melting point, but rather a decomposition starting at approx. 200 °C in Potassium sorbate provides compelling evidence that the conduct of mass spectrometry is technically not feasible for this substance.

In conclusion, apart from the <sup>1</sup>H-NMR spectrum, the determination of spectra specifically for Potassium sorbate is either scientifically unjustified or technically not feasible. Thus, the submission of such spectra is not considered to be required.

	Evaluation by Competent Authorities
,	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE (*)
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	
	COMMENTS FROM
Date	
Evaluation of applicant's justification	
Conclusion	
Remarks	

	Sorbic acid M	arch 2004
	Р	age 1 of 1
Section A3.11 Annex Point IIA3.8	Flammability, including auto-flammability and identity of combustion products  - Flammability in contact with water -  - Pyrophoric properties -	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ]	Technically not feasible     Scientifically unjustified	
Limited exposure [ ]	Other justification [ ]	
Detailed justification:	Experimental data are not submitted since these are considered to be scientifically unjustified:	
	Flammability in contact with water:	
	From the structural formula and the composition of the substance it can be safely concluded that the substance does not evolve any flammable gases in contact with water or humid air.	
	Pyrophoric properties:	
	From the structural formula and composition of the substance it can be concluded that the substance is stable at room temperature air an is not pyrophoric.	
Undertaking of intended data submission		

	Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE (*)	
Date		
Evaluation of applicant's justification		
Conclusion		
Remarks		
	COMMENTS FROM	
Date		
Evaluation of applicant's justification		
Conclusion		
Remarks		