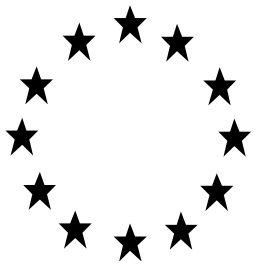
Competent Authority Report



ADDENDUM to Document IIIA, Section 3

Study Summaries Active Substance

C_{8-18}-TMAC
(CAS no. 61789-18-2)

Product-type 8
(Wood Preservatives)

Rapporteur Member State: Italy

May 2014

This Addendum supplements Doc. IIIA Section 3 of the First Draft Competent Authority Report (CAR) which was prepared by the RMS (Italy) according to Directive 98/8/EC for the purpose of the review of the existing biocidal active substance **Quaternary ammonium compounds, coco alkyltrimethyl, chlorides** (C_{8-18}-TMAC, CAS number 61789-18-2) as Wood Preservative (Product Type 8).

This Addendum presents a revised version of the physico-chemical properties table, including the results from the study reports submitted by Akzo Nobel Surface Chemistry AB in May 2012 in order to fill the data gaps which had been remarked by the RMS following the evaluation of the original dossier.

New results have been pointed out in yellow by the Applicant. The RMS-IT conclusions, resulting from the evaluation of the new documentation, are available under the relevant evaluation boxes.

SECTION A3: PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE INGREDIENT

Section A3	A3 Physical and Chemical Properties of Active Substance							For official use only
Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.1 Melting point, boiling point, relative density								
3.1.1 Melting point	OECD 113 and Directive 92/69/EEC, A.1 - DSC method	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	Two DSC-measurements in closed glass crucibles with the test item showed endothermic effects in the temperature ranges 35 - 80 °C, 225 - 270 °C (double peak) and 305 - 320 °C and no exothermal effects up to the maximum test temperature of 400 °C.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Thermal stability (OECD 113) auto flammability A16, Siemens AG Germany, report number 20080278.01, 23oct2008	
3.1.1 Melting point	OECD 102 and Directive 92/69/EEC, A.1 – DSC method	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	The melting point / melting range was determined using a capillary tube in a metal block apparatus. It was not possible to obtain two independent measurements within ± 0.3 K. The lowest begin of melting of the test item TMAC (=Iyophilised Arquad C-35) in the first cycle was determined to be 200 ·C. During three further repetitions a constant melting temperature was not observed. This indicates decomposition during the melting process. This conclusion was confirmed by the fact that the test item changed its colour to brown during the four heating cycles.	Upon request of RMS Italy above study was repeated with observation during heating. The study was terminated because it was impossible to get the repeatable results. It was decided to initiate alternatively a new DSC study was initiated with temperature profile and visual observation between the different temperature trajects. See Moller M 2012.	Y	1	[redacted], 2011, Melting point / melting range, Dr. U. Noack Laboratorien, Germany, Report No.: CPM 14111, 31oct2011 (IIIA3 - TMAC-final report meltingpoint-CPM14111-31oct2011-stamped.pdf)	X

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.1.1 Melting point	(EC A.1., OECD 102)	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	TMAC has no melting point at atmospheric pressure (1013 hPa). The test item decomposes firstly at a temperature > 160 °C.	Upon request of RMS study was repeated because submitted results were not acceptable. The initial initiated capillary method was terminated see above. Alternatively a new DSC study was initiated with temperature profile and visual observation between the different temperature trajects.	Y	1	[redacted], 2012, Determination of physico-chemical properties Thermal Stability (OECD 113) Melting Point (EC A.1., OECD 102) Boiling Point (EC A.2., OECD 103), consilab Gesellschaft für Anlagensicherheit mbH Industriepark Höchst, G 830/840 65926 Frankfurt am Main Germany, Report No.: CSL-11-650.01, 3apr2012 (IIIA3 - TMAC-final report meltingpoint-CSL-11-0650-01-3apr2012-stamped.pdf)	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.1.2 Boiling point	OECD 113 and Directive 92/69/EEC, A.2 - DSC method	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	No mp observed with DCS. Decomposes above 180 °C. (Expected outcome, based on results from lyophilised product: C_{12-16}-TMAC, C_{12-16}-BKC and DDAC)	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Thermal stability (OECD 113) auto flammability A16, Siemens AG Germany, report number 20080278.01, 23oct2008	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.1.2 Boiling point	(EC A.2., OECD 103)	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	TMAC has no boiling point at atmospheric pressure (1013 hPa). The test item decomposes firstly at a temperature > 160 °C.	Upon request of RMS study was repeated because submitted results were not acceptable. The initial initiated capillary method was terminated see above. Alternatively a new DSC study was initiated with temperature profile and visual observation between the different temperature trajects.	Y	1	[redacted], 2012, Determination of physico-chemical properties Thermal Stability (OECD 113) Melting Point (EC A.1., OECD 102) Boiling Point (EC A.2., OECD 103), consilab Gesellschaft für Anlagensicherheit mbH Industriepark Höchst, G 830/840 65926 Frankfurt am Main Germany, Report No.: CSL-11-650.01, 3apr2012 (IIIA3 - TMAC-final report meltingpoint-CSL-11-0650-01-3apr2012-stamped.pdf)	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.1.3 Bulk density/ relative density	OECD 109 and Directive 92/69/EEC method A.3.	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The density of the test item TMAC was determined to be 0.9355 g/cm3 corresponding to 935.5 kg/m3. The relative density solid D20,4 = 0.9355	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5. Ongoing study.	Y	1	[redacted], 2008, Determination of density / relative density, Dr. U. Noack Laboratorien, Germany, Report No.: CPD 12261, 22oct2008	

Section A3	A3 Physical and Chemical Properties of Active Substance							For official use only
Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.2 Vapour pressure	Estimated: (EpiWin v.3.20)	C_{8-18}-TMAC 100% Estimations for the individual chains separately.	VP estimations for 25°C, in Pa (between brackets: mm Hg): C_8 : 2,88E-07 (3,84E-05) C_{10}: 5,22E-08 (6,96E-06) C_{12}: 9,27E-09 (1,24E-06) C_{14}: 1,62E-09 (2,16E-07) C_{16}: 2,80E-10 (3,73E-08) C_{18}: 5,35E-11 (7,13E-09) VP estimations for 20°C C_8 : 1,29E-07 (1,72E-05) C_{10}: 2,25E-08 (3,00E-06) C_{12}: 3,85E-09 (5,13E-07) C_{14}: 6,48E-10 (8,64E-08) C_{16}: 1,08E-10 (1,44E-08) C_{18}: 2,00E-11 (2,67E-09)	According to TGD on data requirements the vapour pressure needs not to be measured if calculations indicate that the value is significantly less than 10^{-5} Pa. For all chain lengths individually, the estimated vp are (far) below the mentioned 10^{-5} Pa. Only for C_8 which is the smallest fraction in C_{8-18}-TMAC, the estimated vp is a little over 10^{-5} Pa. Actual determination of vp of C_{12-16}-TMAC resulted to vp (1.8E-10 Pa at 20°C) several orders of magnitude lower than the corresponding EpiWin estimations for its chain lengths fractions. Consequen tly, the average vp is very low, and no vp determination is required.	n.a.	2	EpiWin v3.20, 2008, Estimations/calculati ons on C8-18-TMAC, Akzo Nobel Surface Chemistry AB.	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.2 Vapour pressure	European Community (EC), EC no. 761/2009, Part A: Methods for the Determination of Physico-Chemical Properties, Guideline A.4: "Vapour Pressure", Official Journal of the European Union no. L220, August 24, 2009	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	*By isothermal thermogravimetry:* *vp at 20°C: < 1.5 x10-3 Pa* *(< 1.1 x 10-5 mmHg)* *vp at 25°C: < 5.8 x10-3 Pa* *(< 4.3 x 10-5 mmHg)*	Upon request of RMS Italy the vapour pressure was determined because the submitted calculation *(EpiWin v3.20, 2008)* was not acceptable.	Y	1	[redacted], 2012, Determination of vapour pressure of C12-16 BKC by isothermal thermogravimethry, Notox bv The Netherlands, Notox project 202844_499393-3apr2012 (IIIA3 - TMAC-final report vapor pressure 202844_499393-3apr2012-stamped.pdf)	X
3.2.1 Henry´s Law Constant	Estimated: (EpiWin v.3.20)	C_{8-18}-TMAC 100% Estimations for the individual chains separately.	Estimated Henry's Law Constant (HLC) (25°C) in Pa . m^3 . mol^{-1}: C_8 : 4,63E-08 C_{10}: 9,27E-08 C_{12}: 1,82E-07 C_{14}: 3,51E-07 C_{16}: 7,31E-07 C_{18}: 1,41E-06	Not applicable, active substance is not volatile	n.a.	2	EpiWin v3.20, 2008, Estimations/calculations on C8-18-TMAC, Akzo Nobel Surface Chemistry AB.	

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Subsection	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Relia-bility**	**Reference**	
	Calculation based on vapour pressure and water solubility	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	*Non-volatile;* *Calculation performed using a weighted molecular weight and* *- Distilled water concentration:* $k_H = < 1.2 \times 10^{-11}$ *atm.m^3/mol* *- Critical micelle concentration* $k_H = < 4.1 \times 10^{-9}$ *atm.m^3/mol*	Upon request of RMS Italy calculation was repeated with measured vapour pressure results because submitted calculation *EpiWin v3.20, 2008,)* was not acceptable.	Y	1	[redacted], 2012, Determination of physic-chemical properties, Notox The Netherlands, project 202844/A - 495714, xx May , 2012 (IIIA3 - TMAC - final report Notox physchem-202844_495714-11may2012-stamped.pdf)	X
3.3 Appearance								
3.3.1 Physical state	EPA OPPTS 830.6303 - Physical State (1996)	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item TMAC appears to be an amorphous, wax-like solid The test item has a tendency to form clumps.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Appearance Physical state, colour and odour, Dr. U. Noack Laboratorien, Germany, Report No.: CAP122611AH, 22oct2008	
3.3.2 Color	EPA OPPTS 830.6302 - Colour (1996)	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item TMAC appears to be an oyster-white coloured solid	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Appearance Physical state, colour and odour, Dr. U. Noack Laboratorien, Germany, Report No.: CAP122611AH, 22oct2008	

Section A3	A3 Physical and Chemical Properties of Active Substance							For official use only
Subsection	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Relia-bility**	**Reference**	
3.3.3 Odor	EPA OPPTS 830.6304 - Odour (1996)	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item TMAC appears to a soapy odour.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Appearance Physical state, colour and odour, Dr. U. Noack Laboratorien, Germany, Report No.: CAP122611AH, 22oct2008	
3.4 Absorption spectra								
3.4.1 UV/VIS	OECD 101	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	No maximum could be determined in the spectra of 1 g/L test item in aqueous neutral and acid solution. In basic medium a small peak at 214 nm (E = 41 L . (mol - cm)") could be determined. The band width of the peak could not be calculated.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, UV/VIS, Dr. U. Noack Laboratorien, Germany, Report No.: CPU12261, 22oct2008	
3.4.2 IR	OECD 101	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item was characterized by IR-spectroscopy. The identity of the test item was confirmed by agreement of the proposed structure with the obtained spectra.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, characterisation of the molecular structure of Arquad C-35 (lyophilised), Allessa Chemie GmbH Germany, B012/2008, 28oct2008	

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Subsection	**Method**	**Purity/ Specification**	**Results**	**Remarks/ Justification**	**GLP (Y/N)**	**Relia-bility**	**Reference**	
3.4.3 NMR	OECD 101	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item was characterized by 1H-, 13C-NMR- spectroscopy. The identity of the test item was confirmed by agreement of the proposed structure with the obtained spectra.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, characterisation of the molecular structure of Arquad C-35 (lyophilised), Allessa Chemie GmbH Germany, B012/2008, 28oct2008	
3.4.4 MS	OECD 101	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item was characterized by mass spectroscopy. The identity of the test item was confirmed by agreement of the proposed structure with the obtained spectra.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, characterisation of the molecular structure of Arquad C-35 (lyophilised), Allessa Chemie GmbH Germany, B012/2008, 28oct2008	
3.5 Solubility in water	OECD Guide-line 105 - Water Solubility (including effects of pH (5-9)	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	OECD 105. The solubility of the test item TMAC was determined using a modified flask method (graduated cylinder method) at 10, 20 and 30 ± 0.5 °C with preincubation at 35 ± 0.5 °C up to a solubility of 1000 g/L. 2.00 ± 0.01 g of the test item TMAC were soluble in 4.0 mL of acidic and basic solutions (pH 4 and 9) and double distilled water resulting in a total volume of 6.1 mL. Under the investigated test conditions the solubility was found to be independent of the temperature. Solubility = 328 g/L.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, water solubility, Dr. U. Noack Laboratorien, Germany, Report No.: CWF 12261, 4nov2008	

Section A3	A3 Physical and Chemical Properties of Active Substance							For official use only
Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.6 Dissociation constant		C_{8-18}-TMAC	Not required (see 3.5 solubility water) pH of 3.66% = 7.4 (pH at maximum solubility in distilled water: ongoing)	Not required - no core data (see BPD, TNsG): Substance is not acidic or alkaline. Water solubility has been determined. TMAC salts are at the whole pH range fully dissociated in water, consisting of ionised cationic surfactant and chloride as counter ion.	Y	1		
3.7 Solubility in organic solvents, including the effect of temperature on solubility	EC A6 - OECD Guide-line 105	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The solubility of TMAC in n-hexane at 10, 20, 30 °C was determined to be 0.02 g/L, in isopropanol at 20, 30 °C was determined to be 568 g/L. The solubility in isopropanol at 10 °C could not be determined with the applied method.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Solubility in organic solvents, Dr. U. Noack Laboratorien, Germany, Report No.: CLF12261, 31oct2008	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.7 Solubility in organic solvents, including the effect of temperature on solubility	EC A6 - OECD Guide-line 105	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	Solubility in g/l isopropanol at 10°C, 20°C, 30°C C8-TMAC: 18.8, 18.5, 18.3 C10-TMAC: 29.6, 29.5, 29.4 C12-TMAC: 380, 393, 394 C14-TMAC: 95.7, 96.8, 97.2 C16-TMAC: 44.1, 44.4, 44.2 C18-TMAC: 5.78, 5.64, 6.01 C18n-TMAC: 26.0, 25.8, 26.4 Sum: 600, 614, 615 n-hexane at 10°C,20°C,30°C C8-TMAC: <5x10-5, <5x10-5, <5x10-5 C10-TMAC: <5x10-5, <5x10-5, <5x10-5 C12-TMAC: <5x10-5, <5x10-5, 1.18x10-4 C14-TMAC: <1x10-5, <1x10-5, 4.39x10-5 C16-TMAC: <2x10-5, <2x10-5, <2x10-5 C18-TMAC: <2x10-5, <2x10-5, <2x10-5 C18n-TMAC: <1.41x10-5, <1.41x10-5, <1.41x10-5 Sum: <2.14x10-4, <2.14x10-4, <2.14x10-4 n-octanol at 20°C C8-TMAC: 12.7 C10-TMAC: 18.6 C12-TMAC: 109 C14-TMAC: 49.6 C16-TMAC: 26.8 C18-TMAC: 4.45 C18n-TMAC: 21.2 Sum: 243	Upon request of RMS Italy study was repeated because submitted study (Bodsch, 2008) was not acceptable. Solubility in n-octanol was measured at 20 C (for Log Po/w calculation) and solubility in n-hexane and iso-propanol at 10 °C, 20 °C and 30°C	Y	1	[redacted], 2012, Determination of physic-chemical properties, Notox The Netherlands, project 202844/A - 495714, xx May , 2012 (IIIA3 - TMAC - final report Notox physchem-202844_495714-11may2012-stamped.pdf)	X

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products				Not required - no core data (TNsG) as biocidal product as manufactured does not contain organic solvents.)				
3.9 Partition coefficient n-octanol/water	Calculation according to Hansch & Leo (Directive 92/69/EEC method A8)	C_{8-18}-TMAC 100%	Result: 0.66	Calculated according to EC guidelines. Estimation based on C_{8-18}-TMAC with the typical chain length distribution. (Arquad C = C_{8-18}-TMAC 35% a.s. in water)	N	2	[redacted], 1996, Log Po/w for Arquad C calculation results outlined according to EC regulations, Akzo Nobel Deventer, The Netherlands, Report No.: ACRD 968-09, July 16, 1996.	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.9 Partition coefficient n-octanol/water	EC A.8 OECD 107 (Calculation based on solubility in n-octanol and CMC in water)	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	Result at 20°C by calculation from solubility in water and n-octanol: Log Pow : 2.39 n-octanol/critical micelle concentration Log Pow : -0.13 n-octanol/distilled water Log Pow : -0.13 n-octanol/buffer solutions	Upon request of RMS Italy the calculation was repeated with the solubility in n-octanol and the CMC in water	n.a.	1	[redacted], 2012, Determination of physic-chemical properties, Notox The Netherlands, project 202844/A - 495714, xx May , 2012 (IIIA3 - TMAC - final report Notox physchem-202844_495714-11may2012-stamped.pdf) Bodsch J, 2008, Surface tension incl. Determination of CMC, Dr. U. Noack Laboratorien, Germany, Report No.: CPT 122611, 22oct2008	X
3.10 Thermal stability, identity of relevant breakdown products	Directive 92/69/EEC - OECD 113	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	(OECD 113): Two DSC-measurements in closed glass crucibles with the test item showed endothermic effects in the temperature ranges 35 - 80 °C, 225 - 270 °C (double peak) and 305 - 320 °C and no exothermal effects up to the maximum test temperature of 400 °C.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Thermal stability (OECD 113) auto flammability A16, Siemens AG Germany, report number 20080278.01, 23oct2008	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.10 Thermal stability, identity of relevant breakdown products	Storage stability - Effects of temperature Cipac MT 46.3	C_{8-18}-TMAC 35% in water	No significant changes of appearance, pH value, alkalinity and content (C8-C18) of the active ingredients of TMAC were observed after 14 days of storage at 50 ± 2 °C.		Y	1	[redacted], 2008, Accelerated storage procedure, Dr. U. Noack Laboratorien, Germany, Report No.: CPL 12237, 31oct2008	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.10 Thermal stability, identity of relevant breakdown products	OECD 113	C_{8-18}-TMAC 98.4% (Dehydrated TMAC test facility code 14111)	Thermal stability The test item TMAC showed a first endothermic effect in the temperature range 40 - 80 °C. In the temperature range of 1 60 - 210 °C an exothermal effect could be observed, directly followed by a second endothermic effect in the temperature range of 210 - 250 °C, directly followed by a second exothermal effect in the temperature range of 250 - 360 °C.		Y	1	[redacted], 2012, Determination of physico-chemical properties Thermal Stability (OECD 113) Melting Point (EC A.1., OECD 102) Boiling Point (EC A.2., OECD 103), consilab Gesellschaft für Anlagensicherheit mbH Industriepark Höchst, G 830/840 65926 Frankfurt am Main Germany, Report No.: CSL-11-650.01, 3apr2012 (IIIA3 - TMAC-final report meltingpoint-CSL-11-0650-01-3apr2012-stamped.pdf)	X

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.11 Flammability, including auto-flammability and identity of combustion products	Directive 92/69/EEC - Method A10	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The test item TMAC has to be classified as highly flammable.	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, flammability of solids, Dr. U. Noack Laboratorien, Germany, Report No.: CPE 122611, 22oct2008	
	Directive 92/69/ EEC – Method A16	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	(A.16.): No self-ignition temperature was observed up to the maximum test temperature of 405 °C, according to the testing guideline for auto-flammability (solids - determination of relative self-ignition temperature) in the sense of the consolidated version of Council Directive 67/548/EEC Annex V, Method A. 16 (Council Directive 92/69/EEC).	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5.	Y	1	[redacted], 2008, Thermal stability (OECD 113) auto flammability A16, Siemens AG Germany, report number 20080278.01, 23oct2008	
3.12 Flash-point			Not required for solid substances	Not required (TNsG): Test substance is a solid (see 3.3.1) which does not give rise to the forming of vapours. (see 3.2)	N	n.a.		
3.13 Surface tension	OECD 115 and Directive 92/69/ EEC - Method A5	C_{8-18}-TMAC 99.6%% (Dehydrated TMAC test facility code 12261)	The surface tension of TMAC = 24.04 +/- 0.05 mN/m. CMC = 1 g/L	Result is based on purified active substance obtained via dehydration of aqueous solution, stored at RT under P_2O_5..	Y	1	[redacted], 2008, Surface tension incl. Determination of CMC, Dr. U. Noack Laboratorien, Germany, Report No.: CPT 122611, 22oct2008	

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Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
	CIPAC Handbook Volume F, MT 47 (1995)	C_{8-18}-TMAC 33.6% in water (batchnumber 4001093971)	The persistent foaming of 100 mL 4 % TMAC solution of Arquad C-35 (corresponding with 1.4% pure TMAC) was determined . The volume of persistent foam of TMAC was determined to be: 16 mL after 10 seconds, 16 mL after 1 minute, 15 mL after 3 minutes, 14 mL after 12 minutes.	Surfactants in general foam when shaken.	Y	1	[redacted], 2008, persistent foaming, Dr. U. Noack Laboratorien, Germany, Report No.: CFO 12237, 6oct2008	
3.14 Viscosity			Not required for solid substances	not required – no core data (TNsG): Test substance is a solid (see 3.3.1)	n.a.	n.a.		
	OECD 114	C_{8-18}-TMAC 33.6% in water (batchnumber 4001093971)	Kinematic viscosity (mm2/s): 20 °C: 30,2 40 °C: 22,3	Result is based on commercial product Arquad C-35	Y	1	[redacted], 2008, Kinematic viscosity OECD 114, Siemens AG Germany, 20080346.01, 24jul2008	
3.15 Explosive properties	Directive 92/69/ EEC – Method A14	C_{8-18}-TMAC 100% (Dehydrated TMAC)	No explosive properties expected (Expected judgement)	Expert statement under GLP.	Y	1	[redacted], 2008, Statement on explosive properties, Dr. U. Noack Laboratorien, Germany, Report No.: CEP 12261, 22oct2008	

Section A3	A3 Physical and Chemical Properties of Active Substance							For official use only
Subsection	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Relia-bility	Reference	
3.16 Oxidizing properties	Directive 92/69/EC -Method A17	C_{8-18}-TMAC 100% (Dehydrated TMAC)	No oxidising properties expected (Expected judgement)	Expert statement under GLP.	Y	1	[redacted], 2008, Statement on oxidising properties, Dr. U. Noack Laboratorien, Germany, Report No.: CES 12261, 22oct2008	
3.17 Reactivity towards container material		C_{8-18}-TMAC 35% in water	No reactivity anticipated when stored properly in original packaging, only approved packaging material is used.	Results are based on the marketed substance.	N	n.a.	[redacted], 2000, Emballage för farligt gods (packaging material for transport of goods), Hannels Industrier i Falkenberg AB.	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	
Conclusion	
Reliability	
Acceptability	
Remarks	**The physical-chemical studies available in the original dossier have been carried out on lyophilized Arquad C-35 from batch 4001093971 (renamed batch 12261 at test facility after dehydration; purity: 99.6% w/w). Whereas, new physical-chemical tests submitted in May 2012 have been performed on lyophilized Arquad C-35 from a different batch (batch 4001122258). The eCA-IT believes that the C_{8-18}-TMAC purity of the test item newly investigated is not the one stated by the Applicant (i.e. 98.4% w/w, which includes C18-unsaturated TMAC), but 91.9% w/w (ISSUE TO BE DISCUSSED AT WG LEVEL).**
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	**3.1.1 Melting point/02** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 91.9% C_{8-18}-TMAC EC method A.1, OECD 102. Capillary tube in a metal block apparatus. In the main test 3 replicates were tested simultaneously starting at 100 °C (heating rate: max. 1 K/min). The test was repeated 4 times with the same samples.
Conclusion	It was not possible to obtain 2 independent measurements within the range of the estimated accuracy provided for by the above guidelines. Furthermore, the onset of melting was observed at different temperatures with respect to the first cycle, where melting started >200 °C. The test item is suspected to decompose during melting. Also the change of colour (from light-yellowish to brown) during the heating cycles suggests decomposition.
Reliability	1
Acceptability	Acceptable
Remarks	X – it shall be noted that estimated accuracy for the "Capillary tube in a metal block apparatus" is not ±0.3 K (as erroneously indicated in the original study report), but ±0.5 K.
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	**3.1.1 Melting point/03** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 91.9% C_{8-18}-TMAC EC method A.1, OECD 102. Differential Scanning Calorimetry (DSC). Heating/cooling rate: 3 K/min; sample container: glass crucible; reference: empty open glass crucible; test atmosphere: air. Two series of experiments have been performed: 1st series (five measurements): the crucibles were heated from 0°C up to 80, 140, 210, 240 or 300 °C. Once the maximum temperature had been reached, the DSC-apparatus was opened for the visual inspection of the crucible. 2nd series (five measurements): in the first three measurements the crucibles underwent the following temperature cycle: 0 – 80 – 0 –140 – 0 – 210 – 0 °C . In the other two measurements the crucibles were heated from 0 °C up to 240 or 300 °C, then cooled down to 25 °C.
Conclusion	No melting point/range. The test item decomposes above 160 °C, before melting. This conclusion was also confirmed by the results obtained by the capillary method (Büchi melting Point B-540 apparatus; heating rate 10 K/min from 30 °C to 300 °C).
Reliability	1
Acceptability	Acceptable
Remarks	
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	**3.1.1 Boiling point/02** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 91.9% C_{8-18}-TMAC EC method A.2, OECD 103. Differential Scanning Calorimetry (DSC). Heating rate: 3 K/min; sample container: glass crucible; reference: empty open glass crucible; test atmosphere: air. Two series of experiments have been performed: 1st series (five measurements): the crucibles were heated from 0°C up to 80, 140, 210, 240 or 300 °C. Once the maximum temperature had been reached, the DSC-apparatus was opened for the visual inspection of the crucible. 2nd series (five measurements): in the first three measurements the crucibles underwent the following temperature cycle: 0 – 80 – 0 –140 – 0 – 210 – 0 °C. In the other two measurements the crucibles were heated from 0 °C up to 240 or 300 °C, cooled down to 25 °C.
Conclusion	No boiling point/range. The test item decomposes above 160 °C, before melting. This conclusion was also confirmed by the results obtained by the capillary method (Büchi melting Point B-540 apparatus; heating rate 10 K/min from 30 °C to 300 °C).
Reliability	1
Acceptability	Acceptable
Remarks	
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities

EVALUATION BY RAPPORTEUR MEMBER STATE

Date

May 2014

Materials and methods

3.2 Vapour pressure/02

Batch: the test item is lyophilized Arquad C-35 from batch 4001122258.

Purity: 91.9% C_{8-18}-TMAC

OECD 104, EC A.4. Isothermal gravimetric effusion method.

A set of compounds with known vapour pressure was used to determine log $P_{T=20°C}$ *vs.* log $V_{T=20°C}$: benzo(ghi)perylene, chrysene, hexachlorobenzene, naphthalene, water.

Equation: log $P_{T=20°C}$ = 1.14 log $V_{T=20°C}$ + 4.48 (r > 0.99).

According to the original study report, plots of the log V_T at elevated temperatures *vs.* 1/T were used to determine the logarithms of the evaporation rate at 20 °C for each reference substance (data are not shown in the report).

Temperature program for the test substance: 40 to 140 °C; isothermal intervals of 10 min; increment steps of 10 °C. Experiments were performed under a flow of nitrogen and at atmospheric pressure.

The weight loss of the test substance was measured continuously as a function of time and the results of the test were compared with the results of hexachlorobenzene obtained by the validation test.

Conclusion

The isothermal gravimetric effusion method allows the determination of vapour pressure down to 1 E-10 Pa, but in this case only approximate results have been provided ($P_{20°C}$ < 1.5 E-3 Pa; $P_{25°C}$ < 5.8 E-3 Pa). In principle, the study is not acceptable (please, see remarks under **Acceptability**).

Nonetheless, it should be considered that the very same approach was adopted to investigate the vapour pressure of DDAC and C_{12-16}-BKC (PT8; Applicant: EQC), which were discussed at Technical Meeting level in 2013. It shall be noted that Akzo Nobel is a member of EQC and the vapour pressure study on DDAC and C_{12-16}-BKC was carried out by the same laboratory according to the same procedure followed for C_{8-18}-TMAC. Therefore, the RMS-IT believes that the conclusions drawn at TMII2013 for those two structurally-related actives should apply also for C_{8-18}-TMAC for the sake of consistency.

Namely, TMII2013 concluded that, in spite of the methodological and reporting deficiencies of the vapour pressure study, both DDAC and C_{12-16}-BKC are non-volatile. Such conclusion should apply also to C_{8-18}-TMAC. As requested for DDAC and C_{12-16}-BKC, also for C_{8-18}-TMAC the vapour pressure study report should be further amended with the available raw data and with an expert statement on the non-volatility of C_{8-18}-TMAC based on considerations of its structure. It shall be noted that the vapour pressure value is not critical for QUATs such as C_{8-18}-TMAC, since it is not used in the risk assessment.

Reliability

3

Study with major methodological and reporting deficiencies

Acceptability	Not acceptable for the following reasons: 1) According to the guideline, the vapour pressures P_T are calculated from the V_T values by using the linear relationship between the logarithm of the vapour pressure and the logarithm of the evaporation rate. If necessary, an extrapolation to temperatures of 20 and 25°C can be made by regression analysis of log P_T vs. 1/T. In details: The vapour pressure P_T is calculated on the basis of its function of evaporation rate V_T as follows $$\text{Log } P_T = C + D \log V_T$$ where C and D are constants specific for the experimental arrangement used, depending on the diameter of the measurement chamber and on the gas flow rate. These constants must be determined once, by measuring a set of compounds with known vapour pressure and regressing log P_T vs. log V_T. The relationship between the vapour pressure P and the temperature T in Kelvin is given by $$\text{Log } P_T = A + B/T$$ where A and B are constants obtained by regressing log P_T *vs.* 1/T. With this equation, the vapour pressure can be calculated for any other temperature by extrapolation. On the contrary, in [redacted], *Determination of vapour pressure of Coco Alkyltrymethylammonium chloride (TMAC) by isothermal thermogravimetry (Notox project 499393)* a different approach was adopted. Seemingly, the equation described above under **Materials and methods** was not used. The weight loss of the test substance was measured continuously as a function of time and the results of the test were simply compared with the results of hexachlorobenzene obtained by the validation test. The conclusion that $P_{20°C}$ is < 1.5 E-3 Pa and $P_{25°C}$ is < 5.8 E-3 Pa was drawn on the basis that the weight loss of the test substance at 110°C, 120°C, 130°C and 140°C was lower than the weight loss of hexachlorobenzene at the same temperatures. This approach yielded to approximate results. Also note that the procedure adopted is not provided for by EC A.4; no justification for deviating from the guideline was provided in the original study report, either. 2) As described under **Materials and methods** above, for the plot log $P_{T=20°C}$ *vs.* log $V_{T=20°C}$ naphthalene and water were considered, with $P_{T=20°C}$ values of 7.56 and 2.34 E03 Pa, respectively. The method was therefore validated up to 1 E03 Pa, out of the range of 1 E-10 to 1 Pa recommended for the isothermal gravimetric effusion method.
Remarks	It shall be noted that the study was incorrectly referenced in the phys-chem properties table. According to the original study report, the study submitted was performed in compliance with GLP, but the GLP certificate of the test facility was not attached. In the context of DDAC and C_{12-16}-BKC (PT8, EQC) evaluation, the missing GLP certificate was submitted in May 2013 before TM discussion.
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*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	

Evaluation by Competent Authorities

EVALUATION BY RAPPORTEUR MEMBER STATE

Date May 2014

Materials and methods

3.2.1 Henry's law constant/02

Calculated using the following input parameters:

Vapour pressure value at 20°C as available in [redacted], 2012, Determination of vapour pressure of Coco Alkyltrymethylammonium chloride (TMAC) by isothermal thermogravimetry (Notox project 499393): < 1.5 E-3 Pa

Water solubility at 20°C: 328 g/l

Average molecular mass: 272.0 g/mol (re-calculated by the RMS-IT based on the correct alkyl chain lengths distribution, see **Remarks** below)

Conclusion HLC <1.24 E-6 Pa m^3 mol^{-1}

Reliability 0

Acceptability Acceptable

Remarks

The following alkyl chain lengths distribution was provided in the original study report:

Alkyl chain	*TMAC distribution (%)*
C_8	*3.91*
C_{10}	*6.00*
C_{12}	*53.5*
C_{14}	*18.1*
C_{16}	*9.07*
C_{18}	*1.37*
C_{18} *unsat.*	*6.48*

The alkyl chain lengths distribution provided in the original study report is incorrect, since the reported % values correspond to the C8-, C10-, C12-, C14-, C16- and C-18 TMAC % w/w in the investigated test item (lyophilized Arquad C-35 from batch 4001122258). This is confirmed by the fact that the overall sum is not 100% but 98.43%, which is the purity of the a.s. C_{8-18}-TMAC (including C18-unsaturated TMAC) in lyophilized Arquad C-35 .

The correct alkyl chain lengths distribution (re-calculated by RMS-IT) is the following :

Alkyl chain	*TMAC distribution (%)*
C_8	*4.25*
C_{10}	*6.52*
C_{12}	*58.2*
C_{14}	*19.7*
C_{16}	*9.86*
C_{18}	*1.49*

Therefore, the correct average molecular mass to be used in the calculation of the HLC is 272.3 g/mol.

According to the original study report, the study submitted was performed in compliance with GLP, but the GLP certificate of the test facility was not attached. In the context of DDAC and C_{12-16}-BKC (PT8, EQC) evaluation, the missing GLP certificate was submitted in May 2013 before TM discussion.

COMMENTS FROM ...

Date

Results and discussion

Conclusion

Reliability

Acceptability

Remarks

Evaluation by Competent Authorities

EVALUATION BY RAPPORTEUR MEMBER STATE

Date	**May 2014**
Materials and methods	**3.7 Solubility in organic solvents/02** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 91.9% C_{8-18}-TMAC OECD 105, EC A.6 (flask method with LC-MS analysis). Solubility was examined in isopropanol, n-hexane and n-octanol in order to comply with TNsG, which require to consider at least two common solvents with different polarity. **Isopropanol** Preliminary test: the test item was stirred with isopropanol (nominal concentration: 1044 g/l) for 2 days at ca. 20°C; the isopropanol phase was centrifuged, treated and analysed by LC-MS. Main test: nine aliquots of the test item were weighted into glass vessels. To each vessel, isopropanol was added (nominal concentration: 1.01-1.05 g/ml). After magnetic stirring in a thermostatically controlled oven at 10 or 30°C (in a climate room for the test at 20°C) for 24, 48, or 72 hours, the isopropanol phase was centrifuged , treated and analysed by LC-MS. **N-hexane** Preliminary test: the test item was stirred with n-hexane (nominal concentration: 0.550 g/l) for 1 day (2 days for the purpose of C16- and C18-TMAC analysis); the n-hexane phase was centrifuged, treated and analysed by LC-MS. Main test: nine aliquots of the test item were weighted into glass vessels. To each vessel, n-hexane was added (nominal concentration: 52-101 mg/l). After magnetic stirring in a thermostatically controlled oven at 10 or 30°C (in a climate room for the test at 20°C) for 24, 48 and 72 hours, prior to analysis the n-hexane phase was filtered and extracted with the mobile phase used in the LC-MS analytical method . **N-octanol** Preliminary test: the test item was stirred with n-octanol (nominal concentration: 1070 g/l) for 2 days; the n-octanol phase was centrifuged, treated and analysed by LC-MS. Main test: three aliquots of the test item were weighted into glass vessels. To each vessel, n-octanol was added (nominal concentration: 0.705-0.710 g/ml). After magnetic stirring in climate room at 20°C for 24, 48 and 72 hours, the n-octanol phase was centrifuged, treated and analysed by LC-MS.
Conclusion	The Applicant version is adopted only as regards the results in isopropanol and n-octanol. It shall be noted that the results as total C_{8-18}-TMAC should not include C8-unsatured. Solubility in isopropanol as total C_{8-18}-TMAC: 574 g/l at 10°C; 588 g/l at 20°C; 589 g/l at 30°C Solubility in n-octanol as total C_{8-18}-TMAC: 221 g/l at 20°C As far as n-hexane is concerned, results are not acceptable, since the adopted method (flask method) applies to substances with higher solubilities (>E-02 g/l).
Reliability	2 for isopropanol and n-octanol 4 for n-hexane
Acceptability	Acceptable only as far as isopropanol and n-octanol are concerned, since the method adopted is not suitable for the determination of solubilities lower than 1 E-02 g/l. It shall be noted that the **effect of temperature on solubility in n-octanol was not investigated**. **No justification for the non-submission of data has been provided, either.**

Remarks	According to the original study report, the study submitted was performed in compliance with GLP, but the GLP certificate of the test facility was not attached. In the context of DDAC and C_{12-16}-BKC (PT8, EQC) evaluation, the missing GLP certificate was submitted in May 2013 before TM discussion.
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	**3.9 Partition coefficient n-octanol/water / 03** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 91.9% C_{8-18}-TMAC According to OECD 107, in case of surface-active materials such as C_{8-18}-TMAC, Pow can be calculated from individual solubilities in n-octanol and water.
Conclusion	Considering that solubility in n-octanol and water at 20°C is 221 g/l (re-calculated by RMS-IT excluding C18-unsaturated) and 328 g/l, respectively, Pow is calculated to be 0.674 (LogPow = - 0.17). Effect of temperature: solubility in water proved to be independent of temperature, whereas the effect of temperature on n-octanol solubility has not been addressed. Effect of pH: solubility in water proved to independent of pH. The LogPow value is not expected to change with pH. X - The value obtained from solubility in n-octanol and critical micelle concentration will not be taken into account by the RMS.
Reliability	0
Acceptable	Acceptable
Remarks	According to the original study report, the study submitted was performed in compliance with GLP, but the GLP certificate of the test facility was not attached. In the context of DDAC and C_{12-16}-BKC (PT8, EQC) evaluation, the missing GLP certificate was submitted in May 2013 before TM discussion.
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	**May 2014**
Materials and methods	**3.10 Thermal stability, identity of relevant breakdown products** Batch: the test item is lyophilized Arquad C-35 from batch 4001122258. Purity: 92.0% C_{8-18}-TMAC OECD 113 ("Screening test for thermal stability and stability in air"), thermal analysis by DSC (temperature range: RT to 360°C; heating rate: 3 K/min; sample container: closed glass crucible; reference: glass crucible containing aluminium oxide; test atmosphere: nitrogen).
Conclusion	Between room temperature and 150°C, only an endothermic thermal effect was observed (at ca. 30-45 °C), which was neither justified nor further investigated in the original study report. In any case, since no decomposition occurred up to 150 °C, the active substance can be concluded thermally stable.
Reliability	2 (due to incomplete reporting or methodological deficiencies, which do not affect the quality of relevant results)
Acceptability	Acceptable
Remarks	
	COMMENTS FROM ...
Date	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	