Introductory Remarks

Except for information on density and log Pow, no physico-chemical data on Burnt dolomitic lime is provided in this chapter. Where relevant, physical and chemical properties of CaO and MgO are presented instead for the following reasons:

- Dolomitic Lime products of the general formula CaO·MgO do not consist of a fixed Ca/Mg ratio. The content of MgO is variable and ranges from 30 – 36 % w/w.
- The biocidal activity takes place in solution, where it is not possible to distinguish whether dolomitic lime, or a combination of CaO and MgO was added to the matter to be treated.
- The physical and chemical properties of MgO are quite similar to those of CaO. It is expected therefore that the physical chemical properties of CaO·MgO are not differing to an extent which will justify to undertake specific studies on CaO·MgO.

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Not indicated	Not indicated	CaO: 2614 °C MgO: 2852 °C	The values are from three different renowned manuals / standard textbooks. The fact that the values differ from each other indicates that they reflect results from three different experiments (identical values would indicate that there was most likely only one primary publication which was cited by all manuals/ textbooks. Nevertheless, the values are in good agreement. This gives confidence that the experiments were carefully performed.	N	1	(1)	X
	Not indicated	Not indicated	CaO: 2572 °C MgO: 2800 °C		N	1	(2)	
	Not indicated	Not indicated	CaO: 2587 °C MgO: 2642 °C		N	1	(3)	

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1.2 Boiling point	Not indicated	Not indicated	CaO: 2850 °C MgO: 3600 °C	Though the two sources are likely to refer to the same measurements, the indicated values are in line with (i.e. higher than) the melting points. The determination of the exact melting points would have no relevance for the assessment of Burnt dolomitic lime under the BPD.	N	1	(1)(2)	X
3.1.3 Bulk density/ relative density			Density:					X
	Not indicated	Not indicated	CaO: 3,250 – 3,380 kg/m^3 MgO: 3,580 kg/m^3	The same argument as put forward for Section point 3.1.1 applies.	N	1	(1)	
	Not indicated	Not indicated	CaO: 3,320 – 3,350 kg/m^3 MgO: 3,580 kg/m^3		N	1	(2)	
	CIPAC MT186	Neutralac QM: 59.6 % w/w CaO 37.5 % w/w MgO	Pour density: 0.83 g/mL Tap density: 1.15 g/mL		Y	1	Doc. No. 113-006, A3.1.3/07	
	OECD 106 EEC Method A3	Neutralac QM: 59.6 % w/w CaO 37.5 % w/w MgO	Relative density (D_4^{20}) 3.28		Y	1		

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.2 Vapour pressure (IIA3.2)				According to the TNsG on data requirements the "[...] study needs not to be conducted if the melting point is above 300 °C. As the melting points of CaO and MgO lie far above this trigger, the determination of the vapour pressure is not triggered. It can be assumed that the vapour is below 10^{-5} Pa.				
3.2.1 Henry´s Law Constant (Pt. I-A3.2)			not applicable	CaO and MgO are not stable in aqueous systems: They react to $Ca(OH)_2$ and $Mg(OH)_2$. Depending on the burning conditions in the production of CaO MgO, MgO might also not hydrolyse and in this case will consequently be insoluble.				
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Not indicated	Not indicated	CaO: solid MgO: solid CaO/MgO: solid		N N	1 1	(2) (2)	

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.3.2 Colour	Not indicated	Not indicated	CaO: white, grey, yellowish, greyish green or brown (depending on impurities) MgO: white CaO/MgO: white, grey, yellowish, greyish green or brown (depending on impurities)		N	1	(2)	X
3.3.3 Odour				Due to low volatility no odour is expected.				
3.4 Absorption spectra (IIA3.4)								
3.4.1 UV/VIS	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. Recording an UV spectrum is scientifically not necessary for the following reasons: • In the visible region, no absorption of light can be expected, as CaO·MgO does not absorb visible light. This is the reason why it is colourless (white). • In the UV region, absorption of light might be possible. However, it can be predicted that any UV spectrum on Lime variants would not provide information useful for analytical purposes. Please note that the analytical methods for Lime variants are well established. None of them is based on a UV spectrum.							

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.4.2 IR	Selected crystals were cleaved and ground to platelets. Spectra were recorded on a Perkin-Elmer 180 infrared spectrophotometer.	Single crystals of pure MgO or CaO	For CaO and MgO „Multiphonon infrared absorption spectra of MgO and CaO“ are presented in literature. Two main peaks for MgO at 846.5 and 981 cm^{-1} and two main peaks for CaO at 628 and 738 cm^{-1} were found.		N	1	(4)	X

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	Infrared matrix isolation spectroscopy	Test substance $Ca(OH)_2$ was produced in the argon matrix by co-condesation of metallic Ca, water and argon at 15 K on a copper surface. For the test substance Mg(OH)2 a CsI surface was used at 10 K.	For $Ca(OH)_2$ and $Mg(OH)_2$ wavenumbers for the Element-Oxygen asymmetric stretching modes are stated in literature, recorded in the Argon matrix for isolated molecules (591.9 $Ca(OH)_2$ and 866.9 cm^{-1} $Mg(OH)_2$). These values are also interesting, when an IR-spectrum of burnt dolomitic lime is discussed as can be concluded from the following argumentation. The measured frequencies of the metal oxygen stretching mode for any of the mentioned compounds containing Calcium are lower than for those containing Magnesium, because of the higher mass of calcium. The cited values indicate that the metal oxygen stretching mode frequency for calcium containing compounds lies between 590 and 740 cm^{-1}. The magnesium oxygen stretc<hing mode frequencies range from 840 – 990 cm^{-1}. The gap between the two regions allows to distinguish between calcium or magnesium oxygen stretching modes. The cited data is sufficient to assign the peaks in a spectrum of dolomitic lime to the possible vibrational modes.	The test substance was produced *in situ* the argon matrix prior to the measurement. To state a specification of the test substance is therefore not applicable.	N	1	(5) (6)	

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	Absorption spectra measured using CaO powder pressed to various film thicknesses (< 1µm – 6µm)	>99.5%	423 cm^{-1} for MgO, 318 cm^{-1} for CaO see Figure 7 of the cited document.	In addition to the previously submitted multiphonon spectrum, a conventional IR spectrum is submitted.	N	1	(7)	

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	The infrared (IR) absorption spectrum was recorded as a potassium bromide disc over the scan range 4000 to 500 cm^{-1}. Resolution: 4.0 or 8.0 cm^{-1} Number of scans: 64 Gain: 1	Neutralac QM: 58.3 % w/w CaO 38.8 % w/w MgO	For Burnt dolomitic lime a weak sharp peak was observed at 3640 cm^{-1} corresponding to the O-H stretch of $Ca(OH)_2$. A weak broad band at 3450 cm^{-1} was attributed to absorbed H_2O, whereas the weak broad band at 1450 cm^{-1} is attributed to the C-O carbonates stretch.	The IR spectrum was consistent with the assigned structure of the lime variant. Any moisture present will react with CaO to $Ca(OH)_2$ and for this reason, the O-H stretch is also observed in Burnt lime variant. The low intensity of the O-H stretch of the $Ca(OH)_2$ is explained by the larger grain size of the Neutralac QM sample compared to the Precal 30S/N samples. Hence less water is adsorbed onto the surface of the crude Neutralac QM before sample preparation. As described in Document IIIA, section 5, CaO is more reactive than MgO, thus no signal for the O-H stretch of $Mg(OH)_2$ is observed in the IR spectrum of Neutralac QM.	Y	1	Doc. No. 117-001; Section A3.4.2/06 (dossier on Hydrated lime)	
3.4.3 NMR	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. The measurement of Standard ^{13}C-NMR or ^{1}H-NMR spectra for Burnt lime is scientifically not necessary, because there is no carbon or hydrogen in CaO·MgO.							

Section A3 Physical and Chemical Properties of Active Substance (for the components CaO and MgO)

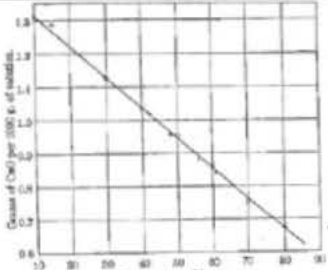
Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.4.4 MS								

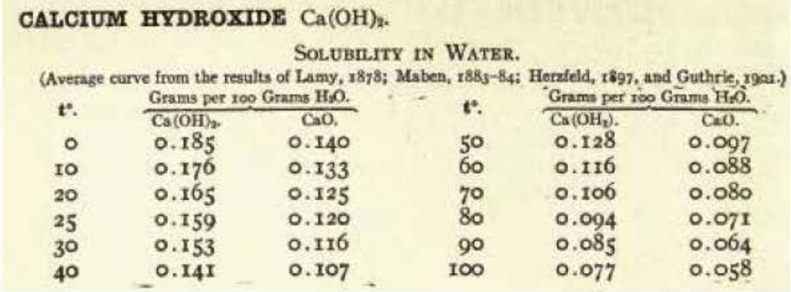
A mass spectrum is not has not been recorded due to the following reasons:

- Only at extremely high temperatures, CaO and MgO peaks could be expected (in consideration of the high melting temperatures).
- The analytical methods for CaO·MgO are well established. None of them is based on an MS spectrum.
- An MS can be calculated (see table)

Table: Expected MS peaks for CaO·MgO.
Values have been calculated on the basis of the abundance of the isotopes of different elements.
Source of model used: http://www2.sisweb.com/mstools/isotope htm

	m / z [u]	Relative intensity of the peaks for the respective fragment related to the highest peak (100).	Assignment
CaO·MgO	56	100	CaO
	58	0.9	
	59	0.1	
	60	2.2	
	64	0.2	
	40	100	MgO
	41	12.6	
	42	14.3	

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.5 Solubility in water (IIA3.5)	Not indicated	Not indicated	CaO: 1.31 g/L cold water 0.7 g/L hot water MgO: 0.0062 g/L cold water 0.086 g/L hot water	CaO and MgO are not stable in aqueous systems: They react to $Ca(OH)_2$ and $Mg(OH)_2$. Depending on the burning conditions in the production of CaO MgO, MgO might also not hydrolyse and in this case will consequently be insoluble. $Ca(OH)_2$ and especially $Mg(OH)_2$ are generally known to be slightly soluble. It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. Cold water refers to water of a temperature close to 0°C and hot water refers to water close the boiling point of 100°C.	N N	1 1	(1) (1)	X
	Not indicated, solubility of lime is expressed as CaO or Ca(OH)2 at different temperatures g/1000 g saturated solution.	Not indicated	 Fig. 1.—Solubility of calcium oxide in water. Circles, [illegible] data; crosses, authors' data.	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity. In this publication, no information on MgO is available.	N	1	(8)	

<table>
<tr><th>Subsection
(Annex Point)</th><th>Method</th><th>Purity/
Specification</th><th>Results
Give also data on test pressure, temperature, pH and concentration range if necessary</th><th>Remarks/
Justification</th><th>GLP (Y/N)</th><th>Relia bility</th><th>Reference</th><th>Official use only</th></tr>
<tr><td rowspan="2"></td><td>Not indicated, solubility of lime is expressed as CaO or $Ca(OH)_2$ different temperatures g/100 g saturated solution.
The conductivity method was used for $Mg(OH)_2$</td><td>Not indicated</td><td>For $Mg(OH)_2$ values for 18°C are given of 0.008 – 0.009 g/L.</td><td rowspan="2">It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature.
It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity.</td><td rowspan="2">N</td><td rowspan="2">1</td><td rowspan="2">(9)</td><td rowspan="2"></td></tr>
<tr><td colspan="3">
CALCIUM HYDROXIDE $Ca(OH)_2$.
SOLUBILITY IN WATER.
(Average curve from the results of Lamy, 1878; Maben, 1883-84; Herzfeld, 1897, and Guthrie, 1901.)
<table>
<tr><th>t°.</th><th>Grams per 100 Grams H_2O.
$Ca(OH)_2$.</th><th>Grams per 100 Grams H_2O.
CaO.</th><th>t°.</th><th>Grams per 100 Grams H_2O.
$Ca(OH_2)$.</th><th>Grams per 100 Grams H_2O.
CaO.</th></tr>
<tr><td>0</td><td>0.185</td><td>0.140</td><td>50</td><td>0.128</td><td>0.097</td></tr>
<tr><td>10</td><td>0.176</td><td>0.133</td><td>60</td><td>0.116</td><td>0.088</td></tr>
<tr><td>20</td><td>0.165</td><td>0.125</td><td>70</td><td>0.106</td><td>0.080</td></tr>
<tr><td>25</td><td>0.159</td><td>0.120</td><td>80</td><td>0.094</td><td>0.071</td></tr>
<tr><td>30</td><td>0.153</td><td>0.116</td><td>90</td><td>0.085</td><td>0.064</td></tr>
<tr><td>40</td><td>0.141</td><td>0.107</td><td>100</td><td>0.077</td><td>0.058</td></tr>
</table></td></tr>
<tr><td>**3.6 Dissociation constant**
(-)</td><td colspan="7">The dissociation constants for CaO and MgO cannot be determined as CaO and MgO react with water to $Ca(OH)_2$ and $Mg(OH)_2$. For $Ca(OH)_2$ and $Mg(OH)_2$ the following information can be provided:</td><td></td></tr>
</table>

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	Not indicated; the thermodynamic quotient of the first ionisation of the base dissolved in aqueous solution at "infinite dilution" is described.	Not indicated	The pH of a saturated $Ca(OH)_2$ solution is 12.4. It can therefore be qualitatively concluded that $Ca(OH)_2$ is a strong base and that pKb < 0. The same holds true for $Mg(OH)_2$. The pK_b of $CaOH^+$ and $MgOH^+$ are 1.2 and 2.6 respectively. It is stated that these forms are very sensitive to ionic medium. MgO reacts with water to $Mg(OH)_2$ which is only slightly soluble in water, hence nearly no dissociation takes place.	It can be assumed that the testing (pH measurement of a saturated $Ca(OH)_2$ solution) was done with the pure substance, as these data come from peer reviewed scientific literature. The basicity of CaO·MgO in water is triggered by the basicity of CaO. pH of a saturated $Ca(OH)_2$ solution is 12.4. $Ca(OH)_2$ and $Mg(OH)_2$ are known to be slightly soluble in water and therefore a direct titration would be hard to conduct.	N	1	(1) (2) (3)	

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.7 **Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	Not indicated	Not indicated	It is expected the CaO·MgO is not soluble in organic solvents. CaO and MgO are not soluble in ethanol. In reference 1 it is stated that they are soluble in acids. It should be noted that CaO reacts exothermically with acids, glycerin and sugarsirups.	There are only qualitative statements on the solubility in ethanol available in literature. It can be assumed that solubility testing was done with the pure substance, as these data come from peer reviewed scientific literature. CaO and MgO are very polar substances. For this reason, it can predicted that they are not soluble in unpolar (= organic) solvents. The fact that CaO and MgO are not soluble in ethanol shows that this statement is valid: please note that ethanol is one of the most polar organic solvents. In less polar organic solvents, CaO can be expected to be less soluble than in ethanol.	N	1	(1) (2)	X
	Shake flask method according to OECD 107	Neutralac QM: 59.6 % w/w CaO 37.5 % w/w MgO	Rate of Calcium recovery in aqueous phase: 103.9 %	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	
3.8 **Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)**			not relevant	There are no formulated products based on Burnt dolomitic lime.				

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.9 Partition coefficient n-octanol/water (IIA3.6)			It is expected, that the logPow is << 3. Burnt dolomitic lime hydrolyses rapidly in water to $Ca(OH)_2$ $Mg(OH)_2$ and/or $Ca(OH)_2MgO$. MgO in $Ca(OH)_2MgO$ has shown to be inert against water and it is therefore insoluble in water and needs not to be considered. No $Ca(OH)_2$ or $Mg(OH)_2$ is dissolved undissociated in water. The portion of $Ca(OH)_2$ and $Mg(OH)_2$ that dissolves in water completely dissociate to Ca^{2+}, Mg^{2+} and OH^-. A test would be performed in buffer solutions at different pH values (5 to 9). Therefore the OH^- concentration is given by the test conditions and only the Ca^{2+} and Mg^{2+} concentration is of relevance. Ca^{2+} and Mg^{2+}, being charged species, are not expected to move to the unpolar n-octanol phase to a significant extent.					X
	OECD 107	Neutralac QM: 59.6 % w/w CaO 37.5 % w/w MgO	Rate of Calcium recovery in aqueous phase: 103.9 % Magnesium concentrations in water prior to testing were very low.	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)			CaO and MgO are stable at extremely high temperatures.	The melting point of CaO is > 2500 °C and of MgO is > 2600 °C. Therefore it can be excluded that CaO·MgO is instable at high temperatures. CaO·MgO is produced from Dolomitic limestone at 900 – 1300 °C. It can be concluded that CaO·MgO is stable at least at this temperature range.				
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)			It can be excluded that CaO·MgO is flammable.	In CaO·MgO, Calcium, Magnesium and Oxygen are in their respective preferred oxidation state. Consequently, flammability can be excluded. Please refer to the arguments provided in the previous point (3.10).				
3.12 Flash-point (IIA3.9)			CaO·MgO is neither capable of burning, nor forming flammable gases.	The same argument as for point 3.11 apply here.				X
3.13 Surface tension (IIA3.10)	OECD 115 EEC A5	90% saturated solution of $Ca(OH)_2$ (98.2 % w/w)	72.5 mN/m	EuLA contracted a study to cover this point with experimental data. The study has been performed with $Ca(OH)_2$ as CaO and MgO hydrolyse rapidly in water to form $Ca(OH)_2$ and $Mg(OH)_2$ anyway. The poor solubility of $Mg(OH)_2$ is not expected to effect the surface tension.	Y	1	Doc. No. 113-001; A3.1.3/02 (dossier on Hydrated lime)	X

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.14 Viscosity **(-)**			not applicable	According to the TNsG this data must only be submitted for liquid substances.				
3.15 Explosive properties (IIA3.11)	According to the TNsG on data requirements „The test can be exempted when [...] absence of certain reactive groups in the structural formula or its "oxygen balance" establishes beyond reasonable doubt that the substance is incapable of decomposing, forming gases or releasing heat very rapidly." These criteria fully apply to CaO·MgO. Please refer to the arguments provided for points 3.10 and 3.11.							
3.16 Oxidizing properties (IIA3.12)	According to the TNsG on data requirements „In cases where an examination of structural formula establishes beyond reasonable doubt that the active ingredient is incapable of reacting exothermically with combustible material, it is acceptable to provide such information as justification for the non-determining of oxidising properties." There is no chemical evidence to assume oxidising properties for CaO·MgO because in CaO·MgO, Calcium, Magnesium and Oxygen are in their respective preferred oxidation state.							
3.17 Reactivity towards container material (IIA3.13)				Experience indicates that paper bags lined with plastic (to prevent contact with moisture), plastic bags, steel, stainless steel and Aluminium do not react significantly with dry lime and so can be used as container material for this product. Aluminium and other materials sensitive to high pH are not suitable container materials for wet lime based products (e.g. milk of lime) For bulk transport of dry lime, steel, stainless steel and Aluminium can be used. Stainless steel is recommended, whereas Aluminium is unsuitable as container materials for bulk transportation of wet lime products.				X

(1) Handbook of Chemistry and Physics, 70th Edition **1989 – 1990**, CRC Press Inc. Boca Raton, Florida. Doc.No. 192-002; Submitted with the Hydrated lime dossier under the Section point A3.1.1/01.

(2) CD Römpp Chemie Lexikon – Version 1.0, Stuttgart/New York: Georg Thieme Verlag **1995**. Doc.No. 192-003; Submitted with the Hydrated lime dossier under the Section point A3.1.3/01.

(3) Hollemann, Wiberg, *“Lehrbuch der anorganischen Chemie”*, 91. – 100. Auflage, de Gruyter, Berlin, New York **1985**. Doc.No. 192-001; Submitted with the Hydrated lime dossier under the Section point A3.1.1/02.

(4) J. T. Gourley and W. A. Runciman*: „Multiphonon infrared absorption spectra of MgO and CaO“*, *J. Phys. C: Solid State Phys.* **1973**, *6*, pp. 583-592. Doc.No. 192-007; Submitted with the Burnt lime dossier under the Section point A3.4.2/03.

(5) J. W. Kauffman, R. H. Hauge, J. L. Margrave: **„***Infrared Matrix Isolation Studies of the Interactions of Mg, Ca, Sr and Ba Atoms and Small Clusters with Water”*, *High Temperature Science* **1984**, *18*, pp. 97-118. Doc.No. 192-004; Submitted with the Hydrated lime dossier under the Section point A3.4.2/02.

(6) T. J. Tague, Jr., L. Andrews: *„Pulsed Laser evaporated Magnesium Atom Reactions with Hydrogen – Infrared Spectra of five Magnesium Hydride Molecules”*, *J. Phys. Chem.* **1994**, *98*, p. 8611. Doc.No. 192-006; A3.4.2/04.

(7) A.M. Hofmeister, E. Keppel and A.K. Speck, *„Absorption and reflection infrared spectra of MgO and other diatomic compounds*“, Mon. Not. R. Astron. Soc**. 2003**, 345, pp. 16-38. Doc. No. 192-009 submitted with the Burnt lime dossier under the Section point A3.4.2/01.

(8) R.T. Haslam, G. Calingaert, C.M. Taylor:” The Hydrates of Lime”, J. Am. Chem. Soc., **1924**, 46 (2), pp. 308-311. Doc. No. 192-010; Submitted with the Hydrated lime dossier under the Section point A3.5/01.

(9) A. Seidell, **1919**, “Solubilities of inorganic and organic substances – a compilation of quatitantive solubility data from the periodical literature”; Stanhope Press. Doc. No. 192-011; Submitted with the Hydrated lime dossier under the Section point A3.5/02.

This statement is to show that irrespective of the Lime variant (Calcium or Dolomitic variants) suspended in water, the solution obtained is always a saturated solution of $Ca(OH)_2$ with negligible traces of Mg^{2+} in solution.
This fact is relevant when studies on the surface tension of the Lime variants are considered. One study with $Ca(OH)_2$ covers the requirements for the studies for all the other variants, for the following reasons:

- Burnt dolomitic lime reacts with water to form $Ca(OH)_2MgO$ or $Ca(OH)_2Mg(OH)_2$. Only the completely hydrated form needs to be considered in detail, as the MgO in $Ca(OH)_2MgO$ has shown to be inert against water and is therefore insoluble. Hence a “solution” of $Ca(OH)_2MgO$ in water is a solution of $Ca(OH)_2$.
- To consider the species in water when $Ca(OH)_2Mg(OH)_2$ is dissolved the solubility products need to be considered (K_L)

$K_L(Ca(OH)_2) = 3.9 \times 10^{-6}$ mol^3 / L^3

$K_L(Mg(OH)_2) = 1.5 \times 10^{-12}$ mol^3 / L^3

On the basis of these solubility products, the solubilities can be calculated as:

$L(Ca(OH)_2) = 9.9$ mmol / L and $L(Mg(OH)_2) = 0.072$ mmol / L

As can be seen the solubility of $Ca(OH)_2$ is ca. 137 times the solubiliy of $Mg(OH)_2$.

In pure water a maximum of 4.2 mg of $Mg(OH)_2$ can dissolve.

The highest possible concentration of Mg^{2+} is calculated for the pH-value of a saturated $Ca(OH)_2$ in the following:

pH = 12.4; $c(OH^-) = 0.025$ mol /L

$K_L(Mg(OH)_2) = c(Mg^{2+}) \times c(OH^-)^2 = c(Mg^{2+}) \times (0.025 \text{ mol /L})^2 = c(Mg^{2+}) \times 0.00063 \text{ mol}^2/L^2$

$c(Mg^{2+}) = 0.00000238$ mmol / L or **0.06 µg / L**

Corresponding of 0.138 µg / L dissolved $Mg(OH)_2$.

It can be concluded that in the presence of $Ca(OH)_2$, i.e. at high pH values, Mg^{2+} concentrations are negligible.

Evaluation by Competent Authorities

Use separate "evaluation boxes" to provide transparency as to the comments and views submitted

EVALUATION BY RAPPORTEUR MEMBER STATE

Date 17 September 2010

Materials and methods Adopt applicant's version with the following amendments.

Some of the data submitted in section 3 are taken from the published literature in the form of well established reference texts which are identified in the reference list. As a result details such as purity of sample and methods used are not available.

However, it is considered that the information supplied is suitable for its intended use especially given that the data have been in use for a considerable time in many technical fields apart from the uses of immediate concern.

The remaining physicochemical tests have been conducted on identified samples and reports have been submitted but the reports are not necessarily to GLP.

The following points are recorded for individual studies.

3.1.1 Melting point
Literature values - Method and purity not recorded. The studies are not to GLP The values quoted are high enough (>2000°C) for the differences to be of little concern. The provision of separate data for Magnesium hydroxide is acceptable. Reliability 2.

3.1.2 Boiling point
Literature values - Method and purity not recorded. The studies are not to GLP The values quoted are high enough (>2000°C) for the differences to be of little concern. The provision of separate data for Magnesium hydroxide is acceptable. Reliability 2.

3.1.3 Relative density
The relative density will vary depending on the source of the lime and the level and identity of the impurities present. The measured value reported is within a range quoted from one of the reference texts.
Reliability of the literature values 2.
The Pycnometer method was used in the study carried out on Neutralac QM.

3.3.2 Colour
In the study reports for Neutralac QM the appearance is recorded as white/beige powder.

3.4.2 IR Spectrum
Details of an infra red spectrum recorded as a potassium bromide disc over the scan range 4000-500 cm-1 (Doc 117-001) are available. The remaining information relating to infra red spectra can be disregarded.

3.5 Solubility in water
Literature values - Method and purity not recorded. The studies are not to GLP.
Document 192-002 (the CRC handbook) gives
CaO: hot-water as 80ºC and cold-water as 10ºC
MgO: hot-water as 30ºC but no temperature given for the cold water value.
Reliability 2.

	3.7 Solubility in organic solvents Limited qualitative data from literature only. The studies are not to GLP Reliability of the literature values 2. Non GLP studies on identified samples measuring the partition coefficient of burnt dolomitic lime indicated that the substance hydrolyses and there is no absorption into the organic layer. 3.9 Partition coefficient n-octanol/water Non GLP studies on identified samples confirm that the partition coefficient of burnt dolomitic lime could not be calculated. The substance hydrolyses. 3.12 Flash point The substance is a solid therefore the determination of flash point is not applicable. 3.13 Surface tension The OECD Harmonised ring method was used. A 1g/L solution was measured rather than a 90% saturated solution of hydrated lime. Burnt lime hydrolyses to hydrated lime. The test was conducted on Hydrated lime. Because of the poor solubility of Magnesium hydroxide a significantly different result is not expected. 3.17 Reactivity towards container material There should be clear evidence that no problems will arise if aluminium is to be used for any product.
Conclusion	Adopt applicant’s version with the above amendments.
Reliability	The following entries are based on recent tests conducted on identified samples. Reliability is 1. 3.1.3 Relative density / Bulk density 3.4 Spectra (IR) 3.7 Solubility in organic solvents 3.9 Partition coefficient 3.13 Surface tension Reliability of the literature values is 2
Acceptability	Acceptable
Remarks	None
	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	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Not indicated Not indicated Not indicated	Not indicated Not indicated Not indicated	2614 °C 2572 °C 2587 °C	The values are from three different renowned manuals / standard textbooks. The fact that the values differ from each other indicates that they reflect results from three different experiments (identical values would indicate that there was most likely only one primary publication which was cited by all manuals/ textbooks. Nevertheless, the values are in good agreement. This gives confidence that the experiments were carefully performed.	N N N	1 1 1	(1) (2) (3)	X
3.1.2 Boiling point	Not indicated Not indicated	Not indicated Not indicated	2850 °C 2850 °C	Though the two sources are likely to refer to the same measurement, the indicated value is in line with (i.e. higher than) the melting point. The determination of the exact melting point would have no relevance for the assessment of Burnt lime under the BPD.	N N	1 1	(1) (2)	X
3.1.3 Bulk density/ relative density	Not indicated Not indicated	Not indicated Not indicated	Density: 3,250 – 3,380 kg/m^3 3,320 – 3,350 kg/m^3	The same argument as put forward for Section point 3.1.1 applies.	N N	1 1	(1) (2)	X

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	CIPAC MT186	Precal 30S: 97.6 % w/w	Pour density: 0.74 g/mL Tap density: 1.04 g/mL		Y	1	Doc. No. 113-003, A3.1.3/04	
		Precal 30N: 96.5 % w/w	Pour density: 0.77 g/mL Tap density: 1.08 g/mL		Y	1	Doc. No. 113-004, A3.1.3/05	
	OECD 106 EEC Method A3	Precal 30S: 97.6 % w/w	Relative density (D_4^{20}) 3.09		Y	1	Doc. No. 113-003, A3.1.3/04	X
		Precal 30N: 96.5 % w/w	Relative density (D_4^{20}) 3.21		Y	1	Doc. No. 113-004, A3.1.3/05	X
3.2 Vapour pressure (IIA3.2)				According to the TNsG on data requirements the "[...] study needs not to be conducted if the melting point is above 300 °C. As the melting point of Burnt lime is far above this trigger, the determination of the vapour pressure is not triggered.				
3.2.1 Henry´s Law Constant (Pt. I-A3.2)			not applicable	CaO is not stable in aqueous solution: It reacts with water forming $Ca(OH)_2$.				
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Not indicated	Not indicated	solid		N	1	(2)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.3.2 Colour	Not indicated	Not indicated	colourless, grey, yellowish, greyish green or brown (depending on impurities)	Pure burnt lime is white. Any tint (see left) is caused by the impurities present.	N	1	(2)	X
3.3.3 Odour			odourless	Burnt lime is not volatile. It can therefore be excluded that it has any odour.				
3.4 Absorption spectra (IIA3.4)								
3.4.1 UV/VIS	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. Recording an UV spectrum is scientifically not necessary for the following reasons: • In the visible region, no absorption of light can be expected, as CaO does not absorb visible light. This is the reason why it is colourless (white). • In the UV region, absorption of light might be possible. However, it can be predicted that any UV spectrum on Lime variants would not provide information useful for analytical purposes. Please note that the analytical methods for Lime variants are well established. None of them is based on a UV spectrum.							
3.4.2 IR	Selected crystals were cleaved and ground to platelets. Spectra were recorded on a Perkin-Elmer 180 infrared spectrophotometer.	Single crystals of pure CaO	For CaO, a multiphonon infrared absorption spectrum is presented in literature. Two main peaks occur at 628 and 738 cm^{-1}.		N	1	(4)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	Absorption spectra measured using CaO powder pressed to various film thicknesses (< 1µm – 6µm)	>99.5%	318 cm^{-1} for CaO see Figure 7 of the cited document.	In addition to the multiphonon spectrum, a conventional IR spectrum is submitted.	N	1	(5)	
	The infrared (IR) absorption spectrum was recorded as a potassium bromide disc over the scan range 4000 to 500 cm^{-1}. Resolution: 4.0 or 8.0 cm^{-1} Number of scans: 64 Gain: 1	Precal 30S: 97.9 % w/w Precal 30N: 97.4 % w/w	For Burnt lime a medium/strong sharp peak was observed at 3640 cm^{-1} corresponding to the O-H stretch of $Ca(OH)_2$. A weak broad band at 3450 cm^{-1} was attributed to absorbed H_2O, whereas the weak broad band at 1450 cm^{-1} is attributed to the C-O carbonates stretch.	The IR spectrum was consistent with the assigned structure of the lime variant. Any moisture present will react with CaO to $Ca(OH)_2$ and for this reason, the O-H stretch is also observed in the Burnt lime variant.	Y	1	Doc. No. 117-001; Section A3.4.2/06 (dossier on Hydrated lime)	X
3.4.3 NMR	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. The measurement of Standard ^{13}C-NMR or ^{1}H-NMR spectra for Burnt lime is scientifically not necessary, because there is no carbon or hydrogen in CaO.							

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
3.4.4 MS	A mass spectrum has not been recorded due to the following reasons:							

A mass spectrum has not been recorded due to the following reasons:

- Only at extremely high temperatures, CaO peaks could be expected (in consideration of the high melting temperature).
- The analytical methods for CaO are well established. None of them is based on an MS spectrum.
- An MS can be calculated (see table)

Table: Expected MS peaks for CaO.
Values have been calculated on the basis of the abundance of the isotopes of different elements.
Source of model used: http://www2.sisweb.com/mstools/isotope htm

	m / z [u]	Relative intensity of the peaks for Calcium oxide related to the highest peak (100).	Assignment
CaO	56	100	CaO
	58	0.9	
	59	0.1	
	60	2.2	
	64	0.2	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)		Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.5	**Solubility in water (IIA3.5)**	Not indicated	Not indicated	1.31 g/L cold water 0.7 g/L hot water	CaO is not stable in aqueous solution: It reacts to $Ca(OH)_2$, which is generally known to be only slightly soluble. It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. Cold water refers to water of a temperature close to 0°C and hot water refers to water close the boiling point of 100°C.	N	1	(1)	X
		Not indicated, solubility of lime is expressed as CaO or Ca(OH)2 at different temperatures g/100 g or 1000 g saturated solution.	Not indicated	See graph and table below	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. It is concluded that the differences between the values	N	1	(6) (7)	

Section A3 Physical and Chemical Properties of Active Substance

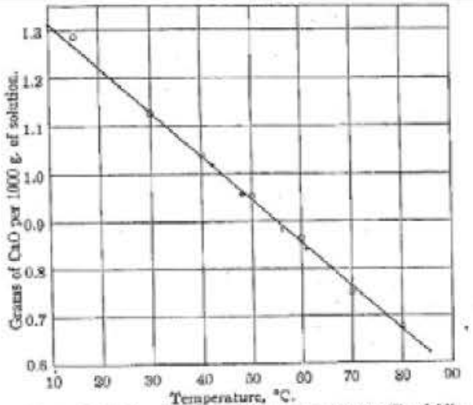
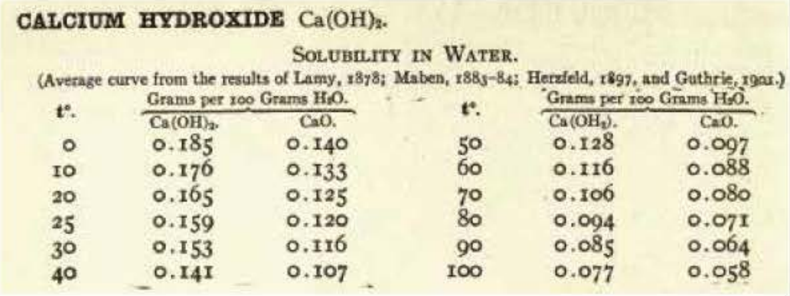
<table>
<tr><th>Subsection
(Annex Point)</th><th>Method</th><th>Purity/
Specification</th><th>Results
Give also data on test pressure, temperature, pH and concentration range if necessary</th><th>Remarks/
Justification</th><th>GLP
(Y/N)</th><th>Relia bility</th><th>Reference</th><th>Official use only</th></tr>
<tr><td></td><td colspan="3">

Fig. 1.—Solubility of calcium oxide in water. Circles, Herzfeld's data; crosses, authors' data.

CALCIUM HYDROXIDE $Ca(OH)_2$.
SOLUBILITY IN WATER.
(Average curve from the results of Lamy, 1878; Maben, 1883-84; Herzfeld, 1897, and Guthrie, 1901.)
<table>
<tr><th>t°.</th><th colspan="2">Grams per 100 Grams H_2O.</th><th>t°.</th><th colspan="2">Grams per 100 Grams H_2O.</th></tr>
<tr><th></th><th>$Ca(OH)_2$.</th><th>CaO.</th><th></th><th>$Ca(OH)_2$.</th><th>CaO.</th></tr>
<tr><td>0</td><td>0.185</td><td>0.140</td><td>50</td><td>0.128</td><td>0.097</td></tr>
<tr><td>10</td><td>0.176</td><td>0.133</td><td>60</td><td>0.116</td><td>0.088</td></tr>
<tr><td>20</td><td>0.165</td><td>0.125</td><td>70</td><td>0.106</td><td>0.080</td></tr>
<tr><td>25</td><td>0.159</td><td>0.120</td><td>80</td><td>0.094</td><td>0.071</td></tr>
<tr><td>30</td><td>0.153</td><td>0.116</td><td>90</td><td>0.085</td><td>0.064</td></tr>
<tr><td>40</td><td>0.141</td><td>0.107</td><td>100</td><td>0.077</td><td>0.058</td></tr>
</table></td><td>can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity.</td><td></td><td></td><td></td><td></td></tr>
<tr><td>3.6 Dissociation constant
(-)</td><td colspan="7">The dissociation constant for CaO cannot be determined as CaO reacts with water to $Ca(OH)_2$ For $Ca(OH)_2$ the following information can be provided:</td><td></td></tr>
</table>

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	Not indicated; the thermodynamic quotient of the first ionisation of the base dissolved in aqueous solution at "infinite dilution" is described.	Not indicated	The pH of a saturated $Ca(OH)_2$ solution is 12.4. It can therefore be qualitatively concluded that $Ca(OH)_2$ is a strong base and that pKb < 0. The pK_b of $CaOH^+$ is 1.2. It is stated that this form is very sensitive to ionic medium.	It can be assumed that the testing (pH measurement of a saturated $Ca(OH)_2$ solution) was done with the pure substance, as these data come from peer reviewed scientific literature. $Ca(OH)_2$ is known to be slightly soluble in water and therefore a direct titration would be hard to conduct.	N	1	(1) (2)	
3.7 **Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	Not indicated	Not indicated	CaO is not soluble in ethanol. In reference 1 it is stated that it is soluble in acids. It should be noted that CaO reacts exothermically with acids, glycerin and sugarsirups.	There is only a qualitative statement on the solubility in ethanol available in literature. It can be assumed that solubility testing was done with the pure substance, as these data come from peer reviewed scientific literature. CaO is a very polar substance. For this reason, it can predicted that it is not soluble in unpolar (= organic) solvents. The fact that CaO is not soluble in ethanol shows that this statement is valid: please note that ethanol is one of the most polar organic solvents. In less polar organic solvents, CaO can be expected to be less soluble than in ethanol.	N	1	(1) (2)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	A shake-flask method was used according to OECD 107	Precal 30S: 97.6 % w/w Precal 30N: 96.5 % w/w	Rate of Calcium recovery in aqueous phase: 102.5 % Rate of Calcium recovery in aqueous phase: 102.9 %	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	X
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)			not relevant	There are no formulated products based on Burnt lime.				
3.9 Partition coefficient n-octanol/water (IIA3.6) log Pow			It is expected, that the logPow is << 3. CaO is slightly soluble in water where it directly transforms to $Ca(OH)_2$ and insoluble in organic solvents. No $Ca(OH)_2$ is dissolved undissociated in water. The portion of $Ca(OH)_2$ that dissolves in water completely dissociates to Ca^{2+} and OH^-.A test would be performed in buffer solutions at different pH values (5 to 9). Therefore the OH^- concentration is given by the test conditions and only the Ca^{2+} concentration is of relevance. Ca^{2+}, being a charged species, is not expected to move to the unpolar n-octanol phase to a significant extent.					X

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	OECD 107	Precal 30S: 97.6 % w/w Precal 30N: 96.5 % w/w	Rate of Calcium recovery in aqueous phase: 102.5 % Rate of Calcium recovery in aqueous phase: 102.9 %	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)			CaO is stable at extremely high temperatures.	The melting point is > 2500 °C. Therefore it can be excluded that CaO is instable at high temperatures. CaO is produced from limestone ($CaCO_3$) at 900 – 1300 °C. It can be concluded that CaO is stable at least at this temperature range.				
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)			It can be excluded that CaO is flammable.	In CaO, Calcium and Oxygen are in their respective preferred oxidation state. Consequently, flammability can be excluded. Please refer to the arguments provided in the previous point (3.10).				
3.12 Flash-point (IIA3.9)			CaO is neither capable of burning, nor forming flammable gases.	The same argument as for point 3.11 applies here.				

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.13 **Surface tension (IIA3.10)**	OECD 115 EEC A5	90% saturated solution of $Ca(OH)_2$ (98.2 % w/w)	72.5 mN/m EuLA has contracted a study to cover this point with experimental data. The study has been performed with $Ca(OH)_2$ as CaO hydrolyses rapidly in water to form $Ca(OH)_2$ anyway.		Y	1	Doc. No. 113-001; A3.1.3/02 (dossier on Hydrated lime)	
3.14 **Viscosity (-)**				According to the TNsG this data need only to be submitted for liquid substances.				
3.15 **Explosive properties (IIA3.11)**	According to the TNsG on data requirements „The test can be exempted when [...] absence of certain reactive groups in the structural formula or its "oxygen balance" establishes beyond reasonable doubt that the substance is incapable of decomposing, forming gases or releasing heat very rapidly.“ These criteria fully apply to CaO. Please refer to the arguments provided for points 3.10 and 3.11.							
3.16 **Oxidizing properties (IIA3.12)**	According to the TNsG on data requirements „In cases where an examination of structural formula establishes beyond reasonable doubt that the active ingredient is incapable of reacting exothermically with combustible material, it is acceptable to provide such information as justification for the non-determining of oxidising properties.“ There is no chemical evidence to assume oxidising properties for CaO because in CaO, Calcium and Oxygen are in their respective preferred oxidation state.							

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.17 Reactivity towards container material (IIA3.13)				Experience indicates that paper bags lined with plastic (to prevent contact with moisture), plastic bags, steel, stainless steel and Aluminium do not react significantly with dry lime and so can be used as container material for this product. Aluminium and other materials sensitive to high pH are not suitable container materials for wet lime based products (e.g. milk of lime) For bulk transport of dry lime, steel, stainless steel and Aluminium can be used. Stainless steel is recommended, whereas Aluminium is unsuitable as container materials for bulk transportation of wet lime products.				

(1) Handbook of Chemistry and Physics, 70th Edition **1989 – 1990**, CRC Press Inc. Boca Raton, Florida. Doc.No. 192-002; Submitted with the Hydrated lime dossier under the Section point A3.1.1/01.

(2) CD Römpp Chemie Lexikon – Version 1.0, Stuttgart/New York: Georg Thieme Verlag **1995**. Doc.No. 192-003; Submitted with the Hydrated lime dossier under the Section point A3.1.3/01.

(3) Hollemann, Wiberg, *"Lehrbuch der anorganischen Chemie"*, 91. – 100. Auflage, de Gruyter, Berlin, New York **1985**. Doc.No. 192-001; Submitted with the Hydrated lime dossier under the Section point A3.1.1/02.

(4) J. T. Gourley and W. A. Runciman*: „Multiphonon infrared absorption spectra of MgO and CaO", J. Phys. C: Solid State Phys.* **1973**, *6*, pp. 583-592. Doc.No. 192-007; A3.4.2/03.

(5) A.M. Hofmeister, E. Keppel and A.K. Speck, „*Absorption and reflection infrared spectra of MgO and other diatomic compounds*“, Mon. Not. R. Astron. Soc**. 2003**, 345, pp. 16-38. Doc. No. 192-009.

(6) R.T. Haslam, G. Calingaert, C.M. Taylor: J. Am. Chem. Soc., **1924**, 46 (2), pp. 308-311. Doc. No. 192-010; Submitted with the Hydrated lime dossier under the Section point A3.5/01.

(7) A. Seidell, **1919**, “Solubilities of inorganic and organic substances – a compilation of quatitantive solubility data from the periodical literature”; Stanhope Press. Doc. No. 192-011; A3.5/02.

Evaluation by Competent Authorities

Use separate "evaluation boxes" to provide transparency as to the comments and views submitted

EVALUATION BY RAPPORTEUR MEMBER STATE

Date 7 September 2010

Materials and methods Adopt applicant's version with the following amendments.

Some of the data submitted in section 3 are taken from the published literature in the form of well established reference texts which are identified in the reference list. As a result details such as purity of sample and methods used are not available.

However, it is considered that the information supplied is suitable for its intended use especially given that the data have been in use for a considerable time in many technical fields apart from the uses of immediate concern.

The remaining physicochemical tests have been conducted on identified samples and reports have been submitted but the reports are not necessarily to GLP.

The following points are recorded for individual studies.

3.1.1 Melting point
Literature values - Method and purity not recorded. The studies are not to GLP
The values quoted are high enough (>2000°C) for the differences to be of little concern.
Reliability 2.

3.1.2 Boiling point
Literature values - Method and purity not recorded. The studies are not to GLP
The values quoted are high enough (>2000°C) for the differences to be of little concern.
Reliability 2.

3.1.3 Relative density
The relative density will vary depending on the source of the lime and the level and identity of the impurities present. The measured values reported are both less than the ranges quoted from in the reference texts.
Reliability of the literature values 2.
In the studies carried out on Precal 30S & Precal 30N the Pycnometer method was used.

3.3.2 Colour
In the study reports for Precal 30N & Precal 30S the appearance is recorded as white/beige powder.

3.4.2 IR Spectrum
Details of an infra red spectrum recorded as a potassium bromide disc over the scan range 4000-500 cm-1 (Doc 117-001) are available. The remaining information relating to infra red spectra can be disregarded.

3.5 Solubility in water
Literature values - Method and purity not recorded. The studies are not to GLP.
Document 192-002 (the CRC handbook) gives hot-water as 80° C and cold-water as 10° C.

Data quoted from documents 192-010 and 192-011 do not refer directly to the

	solubility of calcium oxide. Reliability of other literature values 2. 3.7 Solubility in organic solvents Limited qualitative data from literature only. The studies are not to GLP. Reliability of the literature values 2. Non GLP studies on identified samples measuring the partition coefficient of burnt lime indicated that the substance hydrolyses to hydrated lime and there is no absorption into the organic layer. 3.9 Partition coefficient n-octanol/water Non GLP studies on identified samples confirm that the partition coefficient of burnt lime could not be calculated. Burnt lime hydrolyses to hydrated lime. 3.13 Surface tension The OECD Harmonised ring method was used. A 1g/L solution was measured rather than a 90% saturated solution of hydrated lime. Burnt lime hydrolyses to hydrated lime. 3.17 Reactivity towards container material There should be clear evidence that no problems will arise if aluminium is to be used for any product.
Conclusion	Adopt applicant’s version with the above amendments.
Reliability	The following entries are based on recent tests conducted on identified samples. Reliability is 1. 3.1.3 Relative density / Bulk density 3.4 Spectra (IR) 3.7 Solubility in organic solvents 3.9 Partition coefficient 3.13 Surface tension Reliability of the literature values is 2
Acceptability	Acceptable
Remarks	None
	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	

Introductory Remarks

Hydrated dolomitic lime is produced from Burnt dolomitic lime by reaction with water.

Except for information on density and log Pow, no physico-chemical data on Hydrated dolomitic lime is provided in this chapter. Where relevant, physical and chemical properties of $Ca(OH)_2$ and $Mg(OH)_2$ are presented instead for the following reasons:

- Hydrated dolomitic lime of the general formula $Ca(OH)_2 \cdot Mg(OH)_2$ do not consist of a fixed Ca/Mg ratio. The content of $Mg(OH)_2$ is variable and depends on the MgO content in Burnt dolomitic lime (30 – 36 % w/w).
- The biocidal activity takes place in solution, where it is not possible to distinguish whether Hydrated dolomitic lime, or a combination of $Ca(OH)_2$ and $Mg(OH)_2$ was added to the matter to be treated.
- The physical and chemical properties of $Mg(OH)_2$ are quite similar to those of $Ca(OH)_2$. It is expected therefore that the physical chemical properties of $Ca(OH)_2 \cdot Mg(OH)_2$ are not differing to an extent which will justify to undertake specific studies on $Ca(OH)_2 \cdot Mg(OH)_2$.

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Not indicated	Not indicated	$Ca(OH)_2$: decomposition 580 °C $Mg(OH)_2$: decomposition 350 °C	The values are from three different renowned manuals / standard textbooks. The fact that the values differ from each other indicates that they reflect results from different experiments (identical values would indicate that there was most likely only one primary publication which was cited in all publications. Nevertheless, the values are in fairly good agreement. This gives confidence that the experiments were carefully performed. At decomposition $Ca(OH)_2$ and $Mg(OH)_2$ release water and forms CaO and MgO which have melting points > 2500 °C (refer to the Burnt dolomitic lime dossier DOCIIIA Sec. A3.1.1.).	N	1	(1)	X
	Not indicated	Not indicated	$Ca(OH)_2$: decomposition 450 °C $Mg(OH)_2$: decomposition 380 °C		N	1	(3) (2)	
3.1.2 Boiling point			not applicable	At decomposition $Ca(OH)_2$ and $Mg(OH)_2$ release water and form CaO and MgO which have melting points > 2500 °C (refer to the Burnt dolomitic lime dossier DOCIIIA Sec. A3.1.1.).				

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.1.3 Bulk density/ relative density	Not indicated	Not indicated	Density: $Ca(OH)_2$: 2,240 kg/m^3 $Mg(OH)_2$: 2,360 kg/m^3	The same argument as put forward for Section point 3.1.1 applies.	N	1	(1)	X
	Not indicated	Not indicated	$Ca(OH)_2$: 2,080 – 2,300 kg/m^3 $Mg(OH)_2$: 2,380 kg/m^3		N	1	(2)	
	CIPAC MT186	Neutralac HM: 56.2 % w/w $Ca(OH)_2$ 40.5 % w/w $Mg(OH)_2$	Pour density: 0.38 g/mL Tap density: 0.56 g/mL		Y	1	Doc. No. 113-005, A3.1.3/06	
	OECD 106 EEC Method A3	Neutralac HM: 56.2 % w/w $Ca(OH)_2$ 40.5 % w/w $Mg(OH)_2$	Relative density (D_4^{20}) 2.20		Y	1		X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.2 Vapour pressure (IIA3.2)				According to the TNsG on data requirements the "[...] study needs not to be conducted if the melting point is above 300 °C. It can be assumed that the vapour is below 10^{-5} Pa. $Ca(OH)_2$ and $Mg(OH)_2$ do not melt, but decompose at 450 – 580 °C and 350 – 380 °C, respectively. (See Section point 3.1.1 and 3.1.2).				
3.2.1 Henry´s Law Constant (Pt. I-A3.2)			not applicable	Due to the high decomposition (melting) points of $Ca(OH)_2$ and $Mg(OH)_2$ and therefore low vapour pressure $Ca(OH)_2 \cdot Mg(OH)_2$ as well as $Ca(OH)_2$ and $Mg(OH)_2$ are not expected to evaporate from aqueous solutions.				

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Not indicated	Not indicated	$Ca(OH)_2$: solid $Mg(OH)_2$: solid		N	1	(2) (3)	
3.3.2 Colour	Not indicated	Not indicated	$Ca(OH)_2$: colourless $Mg(OH)_2$: colourless		N	1	(2) (3) (2)	X
3.3.3 Odour	Not indicated	Not indicated	$Ca(OH)_2$: Bitter taste	Due to low volatility of $Ca(OH)_2$ and $Mg(OH)_2$ no odour is expected for $Ca(OH)_2 \cdot Mg(OH)_2$.			(2)	
3.4 Absorption spectra (IIA3.4)								
3.4.1 UV/VIS	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. Recording an UV spectrum is scientifically not necessary for the following reasons: • In the visible region, no absorption of light can be expected, as $Ca(OH)_2 \cdot Mg(OH)_2$ does not absorb visible light. This is the reason why it is colourless (white). • In the UV region, absorption of light might be possible. However, it can be predicted that any UV spectrum on Lime variants would not provide information useful for analytical purposes. Please note that the analytical methods for Lime variants are well established. None of them is based on a UV spectrum.							
3.4.2 IR	No IR-spectrum for Hydrated dolomitic lime was found in literature and therefore a bridging argument is presented based on spectra of $Ca(OH)_2$ and $Mg(OH)_2$ which allows the estimation of an IR-spectrum of Hydrated dolomitic lime.							X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	IR spectra were recorded in KBr using a FTIR-spectrometer (Bruker IFS 88) in a wavenumber range between 600 – 4000 cm^{-1}	The spectrum was recorded with the pure substance.	In figure 1 (see end of table) an IR-spectrum of $Ca(OH)_2$ is presented. The large peak at 3650 cm^{-1} must be assigned to the OH stretching mode. The peak at 1260 – 1410 cm^{-1} must be assigned to OH-deformation mode. The spectrum shown in figure 1 will not be significantly different for $Ca(OH)_2 \cdot Mg(OH)_2$ in the high wavenumber region, because the O-H vibration can be regarded as a molecular vibration, which is only slightly disturbed by neighbouring cations. Furthermore the mass difference between the hydrogen atoms and the rest of the „molecule" is that high, that the frequency of this vibration is practically not influenced by the heavy part of the system. Therefore $Ca(OH)_2$ spectrum can be regarded as a model for O-H stretching modes for any hydroxide containing lime type. If water was involved the peaks assigned to the OH stretching modes would be overlayed by the O-H stretching modes of water. The cited data is sufficient to assign the peaks in a spectrum of a lime variant to the possible vibrational modes.		N	1	(4)	X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	Infrared matrix isolation spectroscopy	Test substance $Ca(OH)_2$ was produced in the argon matrix by co-condesation of metallic Ca, water and argon at 15 K on a copper surface. For the test substance $Mg(OH)_2$ a CsI surface was used at 10 K.	For $Ca(OH)_2$ and $Mg(OH)_2$ wavenumbers for the Element-Oxygen assymetric stretching modes are stated in literature, recorded in the Argon matrix for isolated molecules (591.9 $Ca(OH)_2$ and 866.9 cm^{-1} $Mg(OH)_2$).	The test substance was produced *in situ* the argon matrix prior to the measurement. To state a specification of the test substance is therefore not applicable.	N	1	(5) (6)	X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	The infrared (IR) absorption spectrum was recorded as a potassium bromide disc over the scan range 4000 to 500 cm^{-1}. Resolution: 4.0 or 8.0 cm^{-1} Number of scans: 64 Gain: 1	Neutralac HM: 55.5 % w/w $Ca(OH)_2$ 41.9 % w/w $Mg(OH)_2$	For Hydrated dolomitic lime medium sharp peaks were observed at 3700 cm^{-1} and at 3640 cm^{-1} corresponding to the O-H stretch of $Mg(OH)_2$ and $Ca(OH)_2$, respectively. A weak broad band at 3450 cm^{-1} was attributed to absorbed H_2O, whereas the weak broad band at 1450 cm^{-1} is attributed to the C-O carbonates stretch.	The IR spectrum was consistent with the assigned structure of the lime variant.	Y	1	Doc. No. 117-001; Section A3.4.2/06 (dossier on Hydrated lime)	X
3.4.3 NMR	The measurement of NMR spectra is scientifically not necessary for the following reasons: • A standard ^{13}C-NMR spectrum makes no sense, because there is no carbon in $Ca(OH)_2 \cdot Mg(OH)_2$. • A ^{1}H-NMR spectrum makes no sense because ^{1}H-NMR spectra are usually used as an analytical tool for conformational analysis of organic molecules. No informative result can be expected from a ^{1}H-NMR spectrum of hydrated lime. If the hydrated lime was dissolved in a non protic polar solvent, a peak for the protons might be expected. This would be only one single peak as there are only chemically equivalent protons. • In aqueous solutions the exchange of protons would be extremely fast on the NMR timescale, so that, if at all, only extremely broad peaks can be expected- These would be hardly noticeable/ visible. • The identification techniques for lime are well established and do not utilise NMR spectroscopy.							

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Reliability**	**Reference**	**Official use only**
3.4.4 MS								

To measure mass spectrum of Hydrated dolomitic lime is scientificaly not necessary for the following reason:

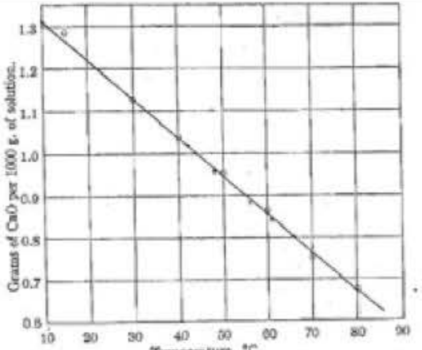
- A mass spectrum is expected not to provide valuable information: Hydrated dolomitic lime would first release water at temperatures up to approx. 500 °C and therefore a water mass spectrum would be observed first. Only at much higher temperatures, CaO and MgO peaks can be expected.
- The analytical methods for Hydrated dolomitic lime are well established. None of them is based on an MS spectrum.

- An MS can be calculated (see table)

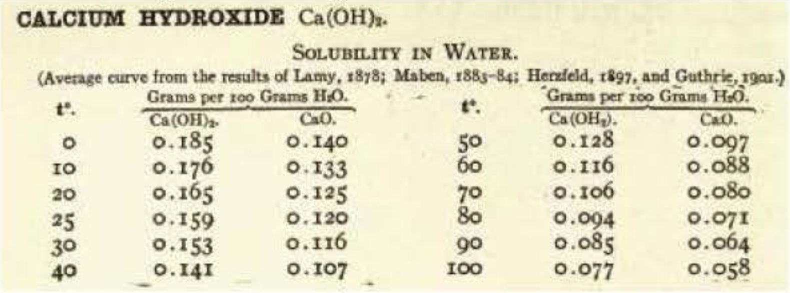
Table: Expected MS peaks for $Ca(OH)_2 \cdot Mg(OH)_2$.
Values have been calculated on the basis of the abundance of the isotopes of different elements.
Source of model used: http://www2.sisweb.com/mstools/isotope htm

	m / z [u]	Relative intensity of the peaks for the respective fragment related to the highest peak (100).	Assignment
$Ca(OH)_2 \cdot Mg(OH)_2$	18	100	H_2O
	20	0.2	
	56	100	CaO
	58	0.9	
	59	0.1	
	60	2.2	
	64	0.2	
	40	100	MgO
	41	12.6	
	42	14.3	

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.5 Solubility in water (IIA3.5)	Not indicated	Not indicated	$Ca(OH)_2$: 1.85 g/L cold water 0.77 g/L hot water	$Ca(OH)_2$ and especially $Mg(OH)_2$ are generally known to be little soluble. It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. Cold water refers to water of a temperature close to 0°C and hot water refers to water close the boiling point of 100°C.	N	1	(1)	X
	Not indicated	Not indicated	$Mg(OH)_2$: 0.009 g/L cold water 0.04 g/L hot water		N	1	(1)	
			$Ca(OH)_2$: 1.26 g/L at 20 °C $Mg(OH)_2$: 0.004 g/L (calculated from solubility of $L(Mg(OH)_2) = 0.72 \cdot 10^{-4}$ mol/L)		N	1	(3)	
	Not indicated, solubility of lime is expressed as CaO at different temperatures g/1000 g saturated solution.	Not indicated	 Fig. 1.—Solubility of calcium oxide in water. Circles, Herzfeld's data; crosses, authors' data.	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity. In this publication no information on $Mg(OH)_2$ is available.	N	1	(8)	X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	Not indicated, solubility of lime is expressed as CaO or $Ca(OH)_2$ different temperatures g/100 g saturated solution. The conductivity method was used for $Mg(OH)_2$	Not indicated	For $Mg(OH)_2$ values for 18°C are given of 0.008 – 0.009 g/L.	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity.	N	1	(9)	X
								

CALCIUM HYDROXIDE $Ca(OH)_2$.

SOLUBILITY IN WATER.

(Average curve from the results of Lamy, 1878; Maben, 1883-84; Herzfeld, 1897, and Guthrie, 1901.)

t°.	Grams per 100 Grams H_2O.		t°.	Grams per 100 Grams H_2O.	
	$Ca(OH)_2$.	CaO.		$Ca(OH_2)$.	CaO.
0	0.185	0.140	50	0.128	0.097
10	0.176	0.133	60	0.116	0.088
20	0.165	0.125	70	0.106	0.080
25	0.159	0.120	80	0.094	0.071
30	0.153	0.116	90	0.085	0.064
40	0.141	0.107	100	0.077	0.058

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.6 Dissociation constant (-)	Not indicated; the thermodynamic quotient of the first ionisation of the base dissolved in aqueous solution at "infinite dilution" is described.	Not indicated	The pH of a saturated $Ca(OH)_2$ solution is 12.4. It can therefore be qualitatively concluded that $Ca(OH)_2$ is a strong base and that $pKb < 0$. The same holds true for $Mg(OH)_2$. The pK_b of $CaOH^+$ and $MgOH^+$ are 1.2 and 2.6 respectively. It is stated that these forms are very sensitive to ionic medium. $Mg(OH)_2$ is only slightly soluble in water, hence nearly no dissociation takes place.	It can be assumed that the testing (pH measurement of a saturated $Ca(OH)_2$ solution) was done with the pure substance, as these data come from peer reviewed scientific literature. The basicity of $Ca(OH)_2 \cdot Mg(OH)_2$ will be triggered by the basicity of $Ca(OH)_2$. pH of a saturated $Ca(OH)_2$ solution is 12.4. $Ca(OH)_2$ and $Mg(OH)_2$ are known to be slightly soluble in water and therefore a direct titration would be hard to conduct.	N	1	(1) (2) (3)	
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Not indicated	Not indicated	Calcium hydroxide is more soluble in glycerine than in water. In reference 1 it is further stated that Calcium hydroxide is soluble in NH_4 salts and acids, insoluble in alcohol. $Mg(OH)_2$ is a polar compound, which is practically not soluble water. It is not expected to be better soluble in organic solvents. In reference 1, Magnesium hydroxide is listed as soluble in NH_4 salts and acids.	It can be assumed that the solubility testing was done with the pure substance, as these data come from peer reviewed scientific literature. The results from literature are in agreement with expectation: Due to its inorganic and polar nature, $Ca(OH)_2 \cdot Mg(OH)_2$ is not expected to be soluble in solvents that are aprotic and less polar than water, in which $Ca(OH)_2$ is slightly and $Mg(OH)_2$ is practically not soluble.	N	1	(1) (2) (9)	X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	Shake flask method according to OECD 107	Neutralac HM: 56.2 % w/w $Ca(OH)_2$ 40.5 % w/w $Mg(OH)_2$	Rate of Calcium recovery in aqueous phase: 103.2 % Magnesium concentrations in water prior to testing were very low.	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)			not relevant	There are no formulated products based on Hydrated dolomitic lime.				
3.9 Partition coefficient n-octanol/water (IIA3.6) log Pow			It is expected, that the logPow is << 3. $Ca(OH)_2$ is slightly soluble in water and insoluble in organic solvents. $Mg(OH)_2$ is more than 2 orders of magnitude less soluble than $Ca(OH)_2$. No $Ca(OH)_2$ or $Mg(OH)_2$ is dissolved undissociated in water. The portion of $Ca(OH)_2$ and $Mg(OH)_2$ that dissolves in water completely dissociates to Ca^{2+}, Mg^{2+} and OH^-. A test would be performed in buffer solutions at different pH values (5 to 9). Therefore the OH^- concentration is given by the test conditions and only the Ca^{2+} and Mg^{2+} concentration is of relevance. Ca^{2+} and Mg^{2+}, being charged species, are not expected to move to the unpolar n-octanol phase to a significant extent.					X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
	OECD 107	Neutralac HM: 56.2 % w/w $Ca(OH)_2$ 40.5 % w/w $Mg(OH)_2$	Rate of Calcium recovery in aqueous phase: 103.2 % Magnesium concentrations in water prior to testing were very low.	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01 (dossier on Hydrated lime)	X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.10 **Thermal stability, identity of relevant breakdown products (IIA3.7)**			$Ca(OH)_2$ decomposes to CaO and water at 580 °C. $Ca(OH)_2$ decomposes to CaO and water at 450 °C. $Mg(OH)_2$ decomposes to CaO and water at 350 °C. $Mg(OH)_2$ decomposes to CaO and water at 380 °C.	$Ca(OH)_2$ and Mg(OH) decompose to CaO, MgO and water (see 3.1.1). Therefore it must be concluded that $Ca(OH)_2{\cdot}Mg(OH)_2$ decomposes to CaO·MgO	N	1	(1) (3) (1) (2)	X
3.11 **Flammability, including auto-flammability and identity of combustion products (IIA3.8)**			It can be excluded that $Ca(OH)_2{\cdot}Mg(OH)_2$ is flammable.	In $Ca(OH)_2{\cdot}Mg(OH)_2$, Calcium, Magnesium and Oxygen are in their respective preferred oxidation state. Consequently, flammability can be excluded.				
3.12 **Flash-point (IIA3.9)**			$Ca(OH)_2{\cdot}Mg(OH)_2$ is neither capable of burning, nor forming flammable gases.	The same argument as for point 3.11 apply here.				X
3.13 **Surface tension (IIA3.10)**	OECD 115 EEC A5	90% saturated solution of $Ca(OH)_2$ (98.2 % w/w)	72.5 mN/m	EuLA has contracted a study to cover this point with experimental data. The study has been performed with $Ca(OH)_2$ as CaO and MgO hydrolyse rapidly in water to form $Ca(OH)_2$ and $Mg(OH)_2$ anyway. The poor solubility of $Mg(OH)_2$ is not expected to effect the surface tension.	Y	1	Doc. No. 113-001; A3.1.3/02 (dossier on Hydrated lime)	X

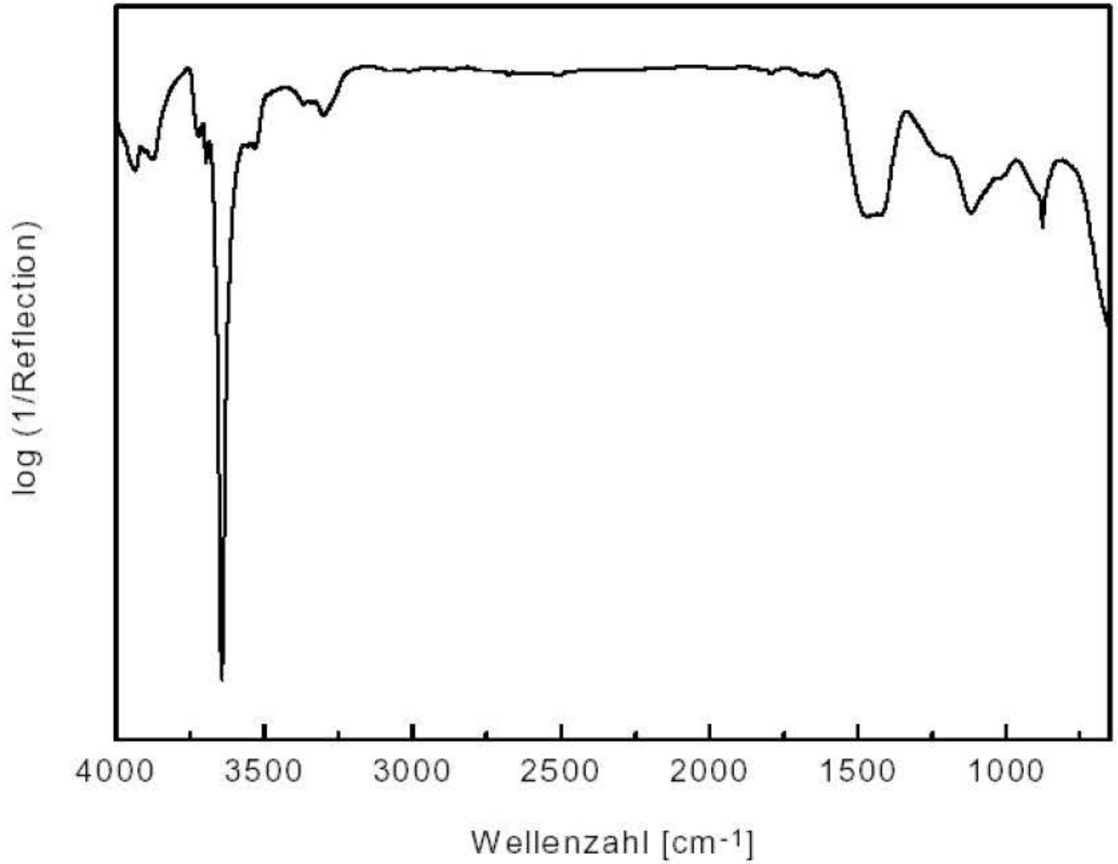
Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
3.14 Viscosity (-)				According to the TNsG this data must only be submitted for liquid substances.				
3.15 Explosive properties (IIA3.11)	According to the TNsG on data requirements „The test can be exempted when [...] absence of certain reactive groups in the structural formula or its "oxygen balance" establishes beyond reasonable doubt that the substance is incapable of decomposing, forming gases or releasing heat very rapidly." These criteria fully apply to $Ca(OH)_2 \cdot Mg(OH)_2$. Please refer to the arguments provided for 3.11.							
3.16 Oxidizing properties (IIA3.12)	According to the TNsG on data requirements „In cases where an examination of structural formula establishes beyond reasonable doubt that the active ingredient is incapable of reacting exothermically with combustible material, it is acceptable to provide such information as justification for the non-determining of oxidising properties." There is no chemical evidence to assume oxidising properties for $Ca(OH)_2 \cdot Mg(OH)_2$ because in $Ca(OH)_2 \cdot Mg(OH)_2$, Calcium, Magnesium and Oxygen are in their respective preferred oxidation state.							

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.17 Reactivity towards container material (IIA3.13)				Experience indicates that paper bags lined with plastic (to prevent contact with moisture), plastic bags, steel, stainless steel and Aluminium do not react significantly with dry lime and so can be used as container material for this product. Aluminium and other materials sensitive to high pH are not suitable container materials for wet lime based products (e.g. milk of lime) For bulk transport of dry lime, steel, stainless steel and Aluminium can be used. Stainless steel is recommended, whereas Aluminium is unsuitable as container materials for bulk transportation of wet lime products.				X

Section A3 **Physical and Chemical Properties of Active Substance (for the components $Ca(OH)_2$ and $Mg(OH)_2$)**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
Figure 1: Infrared spectrum of $Ca(OH)_2$								X

(1) Handbook of Chemistry and Physics, 70th Edition **1989 – 1990**, CRC Press Inc. Boca Raton, Florida. Doc.No. 192-002; Submitted with the Hydrated lime dossier under the Section point A3.1.1/01.

(2) CD Römpp Chemie Lexikon – Version 1.0, Stuttgart/New York: Georg Thieme Verlag **1995**. Doc.No. 192-003; Submitted with the Hydrated lime dossier under the Section point A3.1.3/01.

(3) Hollemann, Wiberg, *“Lehrbuch der anorganischen Chemie”*, 91. – 100. Auflage, de Gruyter, Berlin, New York **1985**. Doc.No. 192-001; Submitted with the Hydrated lime dossier under the Section point A3.1.1/02.

(4) Dirk Lohmann: „Untersuchungen zur Vermeidung zu hoher pH-Werte in weichen Trinkwässern bei der Inbetriebnahme von Rohrleitungen mit einer Zementmörtelauskleidung“, Dissertation, Duisburg. http://www.ub.uni-duisburg.de/ETD-db/theses/available/duett-05212001-095224/unrestricted/inhalt.htm. Doc.No. 192-005; Submitted with the Hydrated lime dossier under the Section point A3.4.2/01.

(5) J. W. Kauffman, R. H. Hauge, J. L. Margrave: **„***Infrared Matrix Isolation Studies of the Interactions of Mg, Ca, Sr and Ba Atoms and Small Clusters with Water”, High Temperature Science* **1984**, *18*, pp. 97-118. Doc.No. 192-004; Submitted with the Hydrated lime dossier under the Section point A3.4.2/02.

(6) T. J. Tague, Jr., L. Andrews: *„Pulsed Laser evaporated Magnesium Atom Reactions with Hydrogen – Infrared Spectra of five Magnesium Hydride Molecules”, J. Phys. Chem.* **1994**, *98*, p. 8611. Doc.No. 192-006; Submitted with the Burnt dolomitic lime dossier under the Section point A3.4.2/04.

(7) J. T. Gourley and W. A. Runciman*: „Multiphonon infrared absorption spectra of MgO and CaO“, J. Phys. C: Solid State Phys.* **1973**, *6*, pp. 583-592. Doc.No. 192-007; Submitted with the Burnt lime dossier under the Section point A3.4.2/03.

(8) R.T. Haslam, G. Calingaert, C.M. Taylor:” The Hydrates of Lime”, J. Am. Chem. Soc., **1924**, 46 (2), pp. 308-311. Doc. No. 192-010; Submitted with the Hydrated lime dossier under the Section point A3.5/01.

(9) A. Seidell, **1919**, “Solubilities of inorganic and organic substances – a compilation of quatitantive solubility data from the periodical literature”; Stanhope Press. Doc. No. 192-011; Submitted with the Hydrated lime dossier under the Section point A3.5/02.

This statement is to show that irrespective of the Lime variant (Calcium or Dolomitic variants) suspended in water, the solution obtained is always a saturated solution of $Ca(OH)_2$ with negligible traces of Mg^{2+} in solution.

This fact is relevant when studies on the surface tension of the Lime variants are considered. One study with $Ca(OH)_2$ covers the requirements for the studies for all the other variants, for the following reasons:

- To consider the species in water when $Ca(OH)_2Mg(OH)_2$ is dissolved the solubility products need to be considered (K_L)

$K_L(Ca(OH)_2) = 3.9 \times 10^{-6}$ mol^3 / L^3

$K_L(Mg(OH)_2) = 1.5 \times 10^{-12}$ mol^3 / L^3

On the basis of these solubility products, the solubilities can be calculated as:

$L(Ca(OH)_2) = 9.9$ mmol / L and $L(Mg(OH)_2) = 0.072$ mmol / L

As can be seen the solubility of $Ca(OH)_2$ is ca. 137 times the solubiliy of $Mg(OH)_2$.

In pure water a maximum of 4.2 mg of $Mg(OH)_2$ can dissolve.

The highest possible concentration of Mg^{2+} is calculated for the pH-value of a saturated $Ca(OH)_2$ in the following:

pH = 12.4; $c(OH^-) = 0.025$ mol /L

$K_L(Mg(OH)_2) = c(Mg^{2+}) \times c(OH^-)^2 = c(Mg^{2+}) \times (0.025 \text{ mol /L})^2 = c(Mg^{2+}) \times 0.00063 \text{ mol}^2/\text{L}^2$

$c(Mg^{2+}) = 0.00000238$ mmol / L or **0.06 µg / L**

Corresponding of 0.138 µg / L dissolved $Mg(OH)_2$.

It can be concluded that in the presence of $Ca(OH)_2$, i.e. at high pH values, Mg^{2+} concentrations are negligible.

Evaluation by Competent Authorities

Use separate "evaluation boxes" to provide transparency as to the comments and views submitted

EVALUATION BY RAPPORTEUR MEMBER STATE

Date 17 August 2010

Materials and methods Adopt applicant's version with the following amendments.

Some of the data submitted in section 3 are taken from the published literature in the form of well established reference texts which are identified in the reference list. As a result details such as purity of sample and methods used are not available.

However, it is considered that the information supplied is suitable for its intended use especially given that the data have been in use for a considerable time in many technical fields apart from the uses of immediate concern.

The remaining physicochemical tests have been conducted on identified samples and reports have been submitted but the reports are not necessarily to GLP.

The following points are recorded for individual studies.

3.1.1 Melting point
Literature values - Method and purity not recorded. The studies are not to GLP
The values quoted are high enough (>360°C) for the differences to be of little concern . The provision of separate data for Magnesium hydroxide is acceptable.
Reliability 2.

3.1.3 Relative density
The relative density will vary depending on the source of the lime and the level and identity of the impurities present. The measured value reported is within a range quoted from one of the reference texts.
Reliability of the literature values 2.
The Pycnometer method was used in the study carried out on Neutralac HM.

3.3.2 Colour
In the study reports for Neutralac HM the appearance is recorded as white/beige powder.

3.4.2 IR Spectrum
Details of an infra red spectrum recorded as a potassium bromide disc over the scan range 4000-500 cm-1 (Doc 117-001) are available. The remaining information relating to infra red spectra can be disregarded.

3.5 Solubility in water
Literature values - Method and purity not recorded. The studies are not to GLP
The reported table is taken from document 192-011 and could be the source of the hot-water and cold-water data from document 192-002 (the CRC handbook) The value of 1.26 g/L at 20°C (taken from document 192-001) appears to have been read from the graph. From the table the value would be 1.65 g/L at 20°C.
Reliability of the literature values 2.

3.7 Solubility in organic solvents
Literature values - Method and purity not recorded. The studies are not to GLP
Reliability of the literature values 2.

3.9 Partition coefficient n-octanol/water
Non GLP studies on identified samples confirm that the partition coefficient of

	hydrated lime could not be calculated. Magnesium Hydroxixe is even less soluble. 3.10 Thermal stability Literature values - Method and purity not recorded. The studies are not to GLP The information is taken from the same sources as the melting point. Calcium hydroxide and magnesium hydroxide do not melt but decompose at elevated temperature. They are thermally stable up to 150°C. Reliability of the literature values 2. 3.12 Flash point The substance is a solid therefore the determination of flash point is not applicable. 3.13 Surface tension The OECD Harmonised ring method was used. A 1g/L solution was measured rather than a 90% saturated solution of hydrated lime. The test was conducted on Hydrated lime. Because of the poor solubility of Magnesium hydroxide a significantly different result is not expected. 3.17 Reactivity towards container material There should be clear evidence that no problems will arise if aluminium is to be used for any product.
Conclusion	Adopt applicant's version with the above amendments.
Reliability	The following entries are based on recent tests conducted on identified samples. Reliability is 1. 3.1.3 Relative density / Bulk density 3.4 Spectra (IR) 3.9 Partition coefficient Reliability of the literature values is 2
Acceptability	Acceptable
Remarks	None
	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	

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	Not indicated Not indicated	Not indicated Not indicated	decomposition 580 °C decomposition 450 °C	The values are from two different renowned manuals / standard textbooks. The fact that the values differ from each other indicates that they reflect results from two different experiments (identical values would indicate that there was most likely only one primary publication which was cited in both publications. Nevertheless, the values are in fairly good agreement. This gives confidence that the experiments were carefully performed. At decomposition $Ca(OH)_2$ releases water and forms CaO which has a melting point > 2500 °C (refer to the Burnt lime dossier Doc IIIA Sec. A3.1.1.).	N N	1 1	(1) (3)	X
3.1.2 Boiling point			not applicable	At decomposition $Ca(OH)_2$ releases water and forms CaO which has a melting point > 2500 °C (refer to the Burnt lime dossier Doc IIIA Sec. A3.1.1.).				

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.1.3 Bulk density/ relative density	Not indicated	Not indicated	Density: 2,240 kg/m^3	The same argument as put forward for Section point 3.1.1 applies.	N	1	(1)	X
	Not indicated	Not indicated	2,080 – 2,300 kg/m^3		N	1	(2)	X
	CIPAC MT186	Precal 50S: 98.2 % w/w	Pour density: 0.45 g/mL Tap density: 0.57 g/mL		Y	1	Doc. No.: 113-001; A3.1.3/02	
		Precal 50N: 97.0 % w/w	Pour density: 0.39 g/mL Tap density: 0.51 g/mL		Y	1	Doc. No.: 113-002; A3.1.3/03	
	OECD 106 EEC Method A3	Precal 50S: 98.2 % w/w	Relative density (D_4^{20}) 2.22		Y	1	Doc. No. 113-001, A3.1.3/02	X
		Precal 50N: 97.0 % w/w	Relative density (D_4^{20}) 2.26		Y	1	Doc. No.: 113-002; A3.1.3/03	X
3.2 Vapour pressure (IIA3.2)				According to the TNsG on data requirements the "[...] study needs not to be conducted if the melting point is above 300 °C. It can be assumed that the vapour is below 10^{-5} Pa. Hydrated lime does not melt, but decomposes at 450 – 580 °C (See Section point 3.1.1 and 3.1.2).				

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.2.1 Henry´s Law Constant (Pt. I-A3.2)				Due to the assumed very low vapour pressure, $Ca(OH)_2$ is not expected to evaporate from aqueous solutions.				
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Not indicated	Not indicated	solid		N	1	(2) (3)	
3.3.2 Colour	Not indicated	Not indicated	colourless, grey, yellowish, greyish green or brown (depending on impurities)	Pure Hydrated lime is white. Any tint (see left) is caused by the impurities present.	N	1	(2) (3)	X
3.3.3 Odour			odourless Bitter taste.	Hydrated lime is not volatile. It can therefore be excluded that it has any odour.			(2)	

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
3.4 Absorption spectra (IIA3.4)								
3.4.1 UV/VIS	According to the TNsG on data requirements, a study needs not to be performed when it is scientifically not necessary. Recording an UV spectrum is scientifically not necessary for the following reasons: • In the visible region, no absorption of light can be expected, as $Ca(OH)_2$ does not absorb visible light. This is the reason why it is colourless (white). • In the UV region, absorption of light might be possible. However, it can be predicted that any UV spectrum on Lime variants would not provide information useful for analytical purposes. Please note that the analytical methods for Lime variants are well established. None of them is based on a UV spectrum.							
3.4.2 IR	IR spectra were recorded in KBr using a FTIR-spectrometer (Bruker IFS 88) in a wavenumber range between 600 – 4000 cm^{-1}	The spectrum was recorded with the pure substance.	In figure 1 (see end of table) an IR-spectrum of $Ca(OH)_2$ is presented. The large peak at 3650 cm^{-1} must be assigned to the OH stretching mode. The peak at 1260 – 1410 cm^{-1} must be assigned to OH-deformation mode.	The pure substance was used to record the IR-spectrum, no further specification on purity or impurities are given. This is acceptable, as it is not expected that impurities would significantly influence the IR spectra of the test substance.	N	1	(4)	X

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
	Infrared matrix isolation spectroscopy	Test substance was produced in the argon matrix by condensation of metallic Ca, water and argon at 15 K on a copper surface	For $Ca(OH)_2$ the wave number for the element-Oxygen asymmetric stretching mode is stated in literature, recorded in the Argon matrix for isolated molecules (591.9 cm^{-1} $Ca(OH)_2$).	The test substance was produced *in situ* the argon matrix prior to the measurement. To state a specification of the test substance is therefore not applicable.	N	1	(5)	X
	The infrared (IR) absorption spectrum was recorded as a potassium bromide disc over the scan range 4000 to 500 cm^{-1}. Resolution: 4.0 or 8.0 cm^{-1} Number of scans: 64 Gain: 1	Precal 50S: 98.4 % w/w Precal 50N: 97.3 % w/w	For $Ca(OH)_2$ a medium/strong sharp peak was observed at 3640 cm^{-1} corresponding to the O-H stretch. A weak broad band at 3450 cm^{-1} was attributed to absorbed H_2O, whereas the weak broad band at 1450 cm^{-1} is attributed to the C-O carbonates stretch.	The IR spectrum was consistent with the assigned structure of the lime variant.	Y	1	Doc. No. 117-001; Section A3.4.2/06	X
3.4.3 NMR	The measurement of NMR spectra is scientifically not necessary for the following reasons: • A standard ^{13}C-NMR spectrum makes no sense, because there is no carbon in $Ca(OH)_2$. • A ^{1}H-NMR spectrum makes no sense because ^{1}H-NMR spectra are usually used as an analytical tool for conformational analysis of organic molecules. No informative result can be expected from a ^{1}H-NMR spectrum of hydrated lime. If the hydrated lime was dissolved in a non protic polar solvent, a peak for the protons might be expected. This would be only one single peak as there are only chemically equivalent protons. • In aqueous solutions the exchange of protons would be extremely fast on the NMR time-scale, so that, if at all, only extremely broad peaks can be expected- These would be hardly noticeable/ visible. • The identification techniques for lime are well established and do not utilise NMR spectroscopy.							

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
3.4.4 MS								

To measure mass spectrum of Hydrated lime is scientifically not necessary for the following reason:

- A mass spectrum is expected not to provide valuable information: Hydrated lime would first release water at temperatures up to approx. 500 °C and therefore a water mass spectrum would be observed first. Only at much higher temperatures, CaO peaks can be expected.
- The analytical methods for CaO are well established. None of them is based on an MS spectrum.
- An MS can be calculated (see table)

Table: Expected MS peaks for Ca(OH)$_2$.
Values have been calculated on the basis of the abundance of the isotopes of different elements.
Source of model used: http://www2.sisweb.com/mstools/isotope htm

	m / z [u]	Relative intensity of the peaks for the respective fragment related to the highest peak (100).	Assignment
Ca(OH)$_2$	18	100	H_2O
	20	0.2	
	56	100	CaO
	58	0.9	
	59	0.1	
	60	2.2	
	64	0.2	

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.5 Solubility in water (IIA3.5)	Not indicated	Not indicated	1.85 g/L cold water 0.77 g/L hot water	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. Cold water refers to water of a temperature close to 0°C and hot water refers to water close the boiling point of 100°C.	N	1	(1)	X
	Not indicated	Not indicated	1.26 g/L at 20 °C	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. The measured water solubility at 20°C is consistent with the results found at 0°C and 100°C, respectively. It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity.	N	1	(3)	X

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	Not indicated, solubility of lime is expressed as CaO or $Ca(OH)_2$ at different temperatures g/100 g or 1000 g saturated solution.	Not indicated	See graph and table below	It can be assumed that the testing was done with the pure substance, as these data come from peer reviewed scientific literature. It is concluded that the differences between the values can be linked to the solvent temperature and it can be assumed that the test substances used were of comparable purity.	N	1	(6) (7)	X

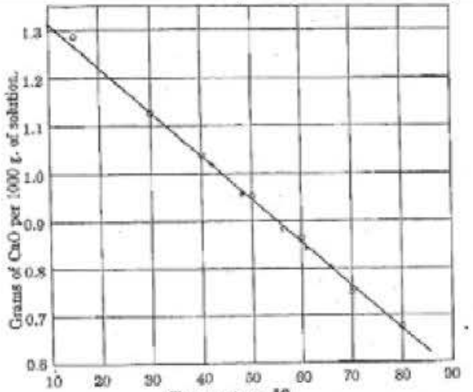
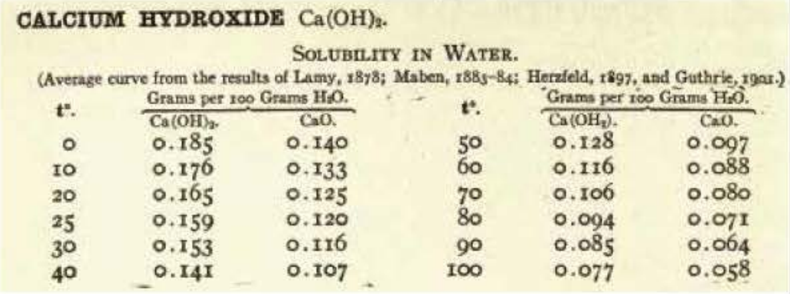


Fig. 1.—Solubility of calcium oxide in water. Circles, Herzfeld's data; crosses, authors' data.



CALCIUM HYDROXIDE $Ca(OH)_2$.

SOLUBILITY IN WATER.

(Average curve from the results of Lamy, 1878; Maben, 1883–84; Herzfeld, 1897, and Guthrie, 1901.)

t°.	Grams per 100 Grams H_2O.		t°.	Grams per 100 Grams H_2O.	
	$Ca(OH)_2$.	CaO.		$Ca(OH_2)$.	CaO.
0	0.185	0.140	50	0.128	0.097
10	0.176	0.133	60	0.116	0.088
20	0.165	0.125	70	0.106	0.080
25	0.159	0.120	80	0.094	0.071
30	0.153	0.116	90	0.085	0.064
40	0.141	0.107	100	0.077	0.058

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.6 **Dissociation constant (-)**	Not indicated; the thermodynamic quotient of the first ionisation of the base dissolved in aqueous solution at "infinite dilution" is described.	Not indicated	The pH of a saturated $Ca(OH)_2$ solution is 12.4. It can therefore be qualitatively concluded that $Ca(OH)_2$ is a strong base and that pKb < 0. The pK_b of $CaOH^+$ is 1.2. It is stated that this form is very sensitive to ionic medium.	It can be assumed that the testing (pH measurement of a saturated $Ca(OH)_2$ solution) was done with the pure substance, as these data come from peer reviewed scientific literature.	N	1	(1) (2)	
3.7 **Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	Not indicated	Not indicated	Calcium hydroxide is more soluble in glycerine than in water. In reference 1 it is further stated that Calcium hydroxide is soluble in NH_4 salts and acids, insoluble in alcohol.	It can be assumed that the solubility testing was done with the pure substance, as these data come from peer reviewed scientific literature. The results from literature are in agreement with expectation: Due to its inorganic and polar nature, Hydrated lime is not expected to be soluble in solvents that are aprotic and less polar than water, in which $Ca(OH)_2$ is only slightly soluble.	N	1	(1) (2) (7)	X
	A shake-flask method was used according to OECD 107	Precal 50S: 98.2 % w/w Precal 50N: 97.0 % w/w	Rate of Calcium recovery in aqueous phase: 102.1 % Rate of Calcium recovery in aqueous phase: 103.1 %	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol	N	1	Doc. No. 154-001; A3.9/01	

Section A3 Physical and Chemical Properties of Active Substance

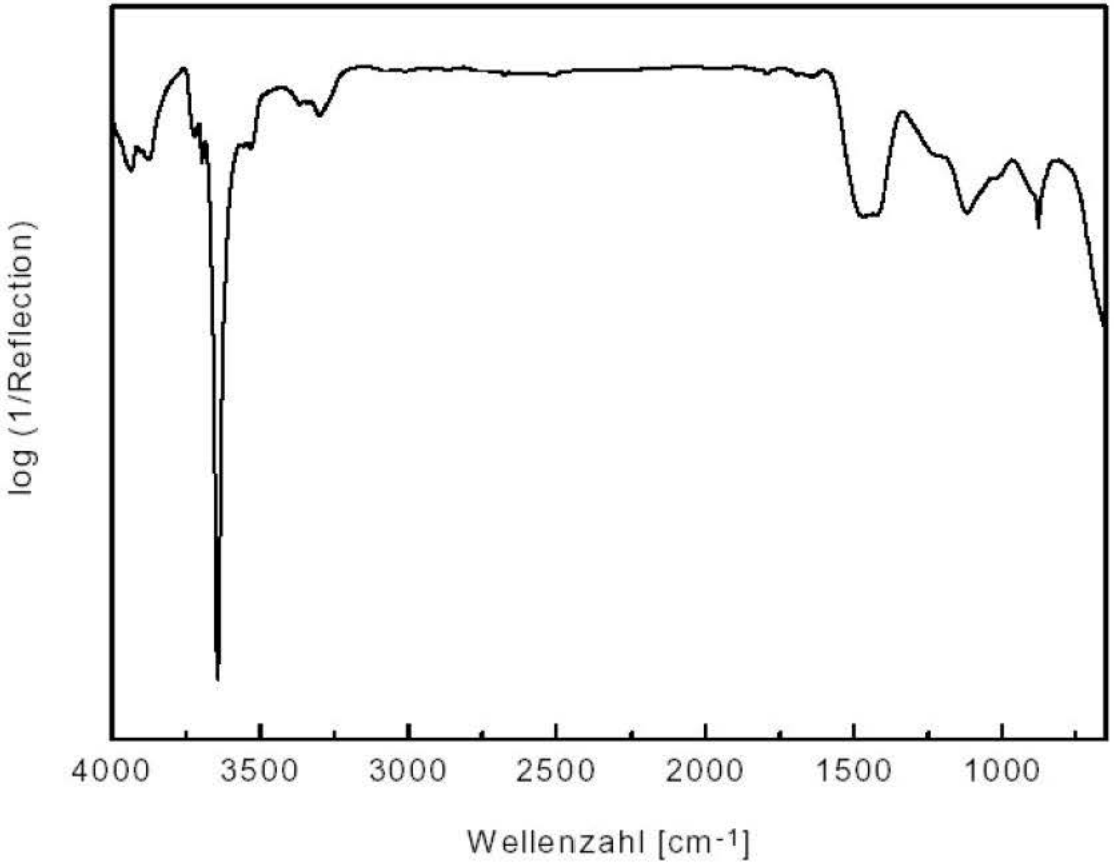
Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.8 **Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)**			not relevant	There are no formulated products based on Hydrated lime.				
3.9 **Partition coefficient n-octanol/water (IIA3.6)**			It is expected, that the logPow is << 3. $Ca(OH)_2$ is slightly soluble in water and insoluble in organic solvents. No $Ca(OH)_2$ is dissolved undissociated in water. The portion of $Ca(OH)_2$ that dissolves in water completely dissociates to Ca^{2+} and OH^-.A test would be performed in buffer solutions at different pH values (5 to 9). Therefore the OH^- concentration is given by the test conditions and only the Ca^{2+} concentration is of relevance. Ca^{2+}, being a charged species, is not expected to move to the unpolar n-octanol phase to a significant extent.					
	OECD 107	Precal 50S: 98.2 % w/w Precal 50N: 97.0 % w/w	Rate of Calcium recovery in aqueous phase: 102.1 % Rate of Calcium recovery in aqueous phase: 103.1 %	The $Ca(OH)_2$-content in the test solutions was completely found in the aqueous phase. $Ca(OH)_2$ does not dissolve in n-octanol and a partition coefficient could therefore not be calculated.	N	1	Doc. No. 154-001; A3.9/01	X

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.10 **Thermal stability, identity of relevant breakdown products (IIA3.7)**	Not indicated	Not indicated	$Ca(OH)_2$ decomposes to CaO and water at 580 °C. $Ca(OH)_2$ decomposes to CaO and water at 450 °C.				(1) (3)	X
3.11 **Flammability, including auto-flammability and identity of combustion products (IIA3.8)**			It can be excluded that $Ca(OH)_2$ is flammable.	In $Ca(OH)_2$, Calcium and Oxygen are in their respective preferred oxidation state. Consequently, flammability can be excluded.				
3.12 **Flash-point (IIA3.9)**			$Ca(OH)_2$ is neither capable of burning, nor forming flammable gases.	The same arguments as for point 3.11 apply here.				
3.13 **Surface tension (IIA3.10)**	OECD 115 EEC A5	90% saturated solution of $Ca(OH)_2$ (98.2 % w/w)	72.5 mN/m		Y	1	Doc. No. 213-001, A3.1.3/02;	X
3.14 **Viscosity (-)**				According to the TNsG this data must only be submitted for liquid substances.				
3.15 **Explosive properties (IIA3.11)**	According to the TNsG on data requirements „The test can be exempted when [...] absence of certain reactive groups in the structural formula or its "oxygen balance" establishes beyond reasonable doubt that the substance is incapable of decomposing, forming gases or releasing heat very rapidly.“ These criteria fully apply to $Ca(OH)_2$. Please refer to the arguments provided for 3.11.							

Section A3 **Physical and Chemical Properties of Active Substance**

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Relia bility	Reference	Official use only
3.16 Oxidising properties (IIA3.12)	According to the TNsG on data requirements „In cases where an examination of structural formula establishes beyond reasonable doubt that the active ingredient is incapable of reacting exothermically with combustible material, it is acceptable to provide such information as justification for the non-determining of oxidising properties.“ There is no chemical evidence to assume oxidising properties for $Ca(OH)_2$ because in $Ca(OH)_2$, Calcium and Oxygen are in their respective preferred oxidation state.							
3.17 Reactivity towards container material (IIA3.13)				Experience indicates that paper bags lined with plastic (to prevent contact with moisture), plastic bags, steel, stainless steel and Aluminium do not react significantly with dry lime and so can be used as container material for this product. Aluminium and other materials sensitive to high pH are not suitable container materials for wet lime based products (e.g. milk of lime) For bulk transport of dry lime, steel, stainless steel and Aluminium can be used. Stainless steel is recommended, whereas Aluminium is unsuitable as container materials for bulk transportation of wet lime products.				X

Subsection (Annex Point)	**Method**	**Purity/ Specification**	**Results** Give also data on test pressure, temperature, pH and concentration range if necessary	**Remarks/ Justification**	**GLP (Y/N)**	**Relia bility**	**Reference**	**Official use only**
Figure 1: Infrared spectrum of $Ca(OH)_2$								

(1) Handbook of Chemistry and Physics, 70th Edition **1989 – 1990**, CRC Press Inc. Boca Raton, Florida. Doc.No. 192-002; A3.1.1/01.

(2) CD Römpp Chemie Lexikon – Version 1.0, Stuttgart/New York: Georg Thieme Verlag **1995**. Doc.No. 192-003; A3.1.3/01.

(3) Hollemann, Wiberg, *“Lehrbuch der anorganischen Chemie”*, 91. – 100. Auflage, de Gruyter, Berlin, New York **1985**. Doc.No. 192-001; A3.1.1/02.

(4) Dirk Lohmann: „Untersuchungen zur Vermeidung zu hoher pH-Werte in weichen Trinkwässern bei der Inbetriebnahme von Rohrleitungen mit einer Zementmörtelauskleidung“, Dissertation, Duisburg. http://www.ub.uni-duisburg.de/ETD-db/theses/available/duett-05212001-095224/unrestricted/inhalt htm. Doc.No. 192-005; A3.4.2/01.

(5) J. W. Kauffman, R. H. Hauge, J. L. Margrave: **„***Infrared Matrix Isolation Studies of the Interactions of Mg, Ca, Sr and Ba Atoms and Small Clusters with Water”*, *High Temperature Science* **1984**, *18*, pp. 97-118. Doc.No. 192-004; A3.4.2/02.

(6) R.T. Haslam, G. Calingaert, C.M. Taylor:” The Hydrates of Lime”, J. Am. Chem. Soc., **1924**, 46 (2), pp. 308-311. Doc. No. 192-010; A3.5/01.

(7) A. Seidell, **1919**, “Solubilities of inorganic and organic substances – a compilation of quatitantive solubility data from the periodical literature”; Stanhope Press. Doc. No. 192-011; A3.5/02.

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted

EVALUATION BY RAPPORTEUR MEMBER STATE

Date 18 June 2010

Materials and methods Adopt applicant's version with the following amendments.

Some of the data submitted in section 3 are taken from the published literature in the form of well established reference texts which are identified in the reference list. As a result details such as purity of sample and methods used are not available.

However, it is considered that the information supplied is suitable for its intended use especially given that the data have been in use for a considerable time in many technical fields apart from the uses of immediate concern.

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The following points are recorded for individual studies.

3.1.1 Melting point
Literature values - Method and purity not recorded. The studies are not to GLP
The values quoted are high enough (>360°C) for the differences to be of little concern.
Reliability 2.

3.1.3 Relative density
The relative density will vary depending on the source of the lime and the level and identity of the impurities present. The measured values reported are within a range quoted from one of the reference texts.
Reliability of the literature values 2.
In the studies carried out on Precal 50S & Precal 50N the Pycnometer method was used.

3.3.2 Colour
In the study reports for Precal 50N & Precal 50S the appearance is recorded as white powder.

3.4.2 IR Spectrum
Details of an infra red spectrum recorded as a potassium bromide disc over the scan range 4000-500 cm-1 (Doc 117-001) are available. The remaining information relating to infra red spectra can be disregarded.

3.5 Solubility in water
Literature values - Method and purity not recorded. The studies are not to GLP
The reported table is taken from document 192-011 and could be the source of the hot-water and cold-water data from document 192-002 (the CRC handbook) The value of 1.26 g/L at 20°C (taken from document 192-001) appears to have been read from the graph. From the table the value would be 1.65 g/L at 20°C.

Reliability of the literature values 2.

3.7 Solubility in organic solvents

	Literature values - Method and purity not recorded. The studies are not to GLP Reliability of the literature values 2. 3.9 Partition coefficient n-octanol/water Non GLP studies on identified samples confirm that the partition coefficient could not be calculated. 3.10 Thermal stability Literature values - Method and purity not recorded. The studies are not to GLP The information is taken from the same sources as the melting point. Hydrated lime does not melt but decomposes at elevated temperature. It is thermally stable up to 150°C. Reliability of the literature values 2. 3.13 Surface tension The OECD Harmonised ring method was used. A 1g/L solution was measured rather than a 90% saturated solution. Document number is incorrect and should read 113-001. 3.17 Reactivity towards container material There should be clear evidence that no problems will arise if aluminium is to be used for any product.
Conclusion	Adopt applicant's version with the above amendments.
Reliability	The following entries are based on recent tests conducted on identified samples. Reliability is 1. 3.1.3 Relative density / Bulk density 3.4 Spectra (IR) 3.9 Partition coefficient 3.13 Surface tension Reliability of the literature values is 2
Acceptability	Acceptable
Remarks	None
	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	