

Sample name: **cs000256**

Experiment start time: **2011-8-31 13:03:34**

Assay name: **pH-metric pKa**

Analyst:

Assay ID: **11H-31007**

Instrument ID:

T311042

Filename: **Y:\1108\11H-31007_cs000256_pH-metric pKa.t3r**

Yasuda-Shedlovsky result

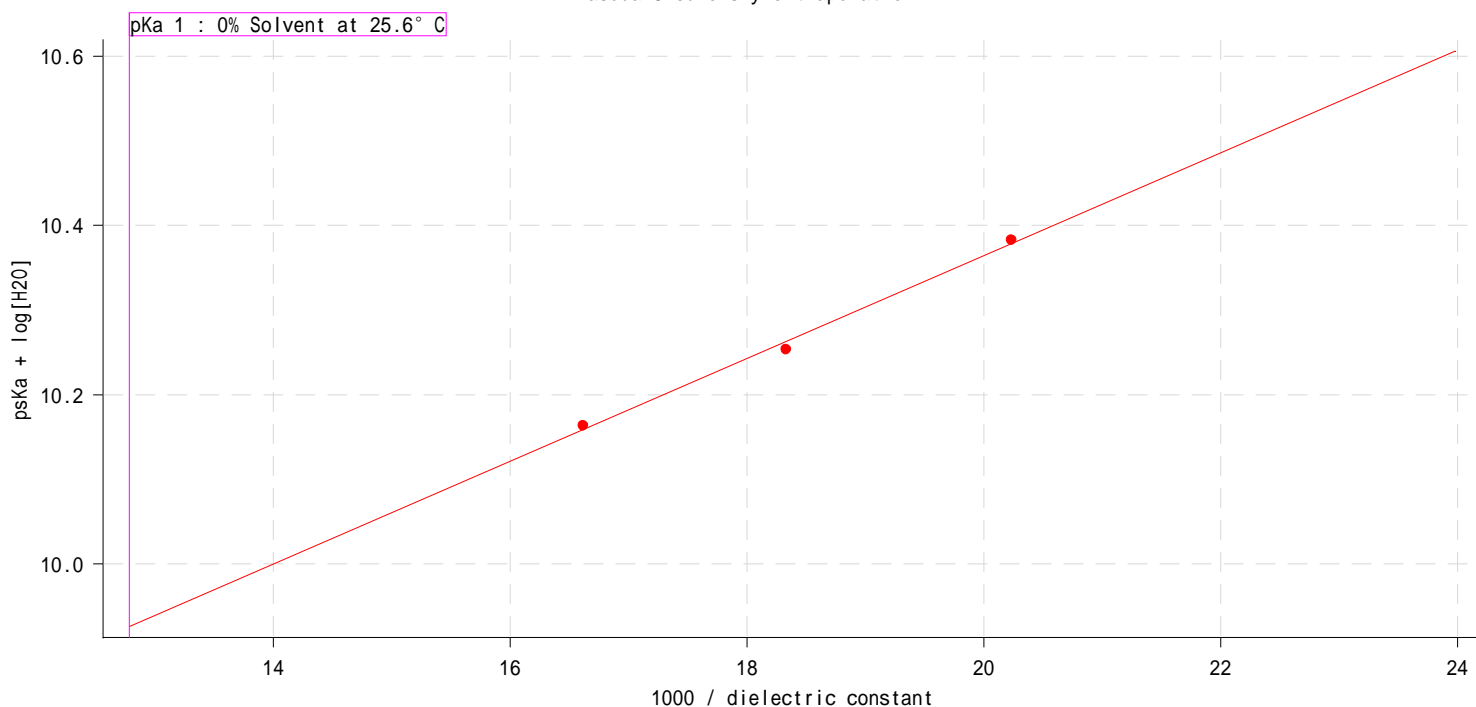
Extrapolation type: **pKa 0%SD** Intercept: **Slope R2** Ionic strength: **Temperature**
Yasuda-Shedlovsky: **8.18 ±0.039.15** **60.68460.99450.171 M** **25.6°C**

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	pKa 1
11H-31007 Points 72 to 109	40.44 %	Up	pH-metric	60.2	29.7 M	0.177 M	26.8°C	✓ 8.69
11H-31007 Points 37 to 71	53.37 %	Up	pH-metric	54.6	22.6 M	0.173 M	25.7°C	✓ 8.90
11H-31007 Points 3 to 36	64.92 %	Up	pH-metric	49.4	16.6 M	0.163 M	24.4°C	✓ 9.16

Graphs

Yasuda-Shedlovsky extrapolation



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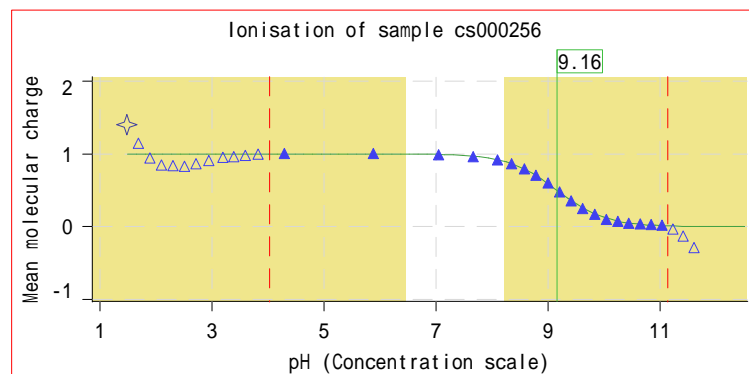
Experiment start time: **2011-8-31 13:03:34**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 311H-31007 Points 3 to 36

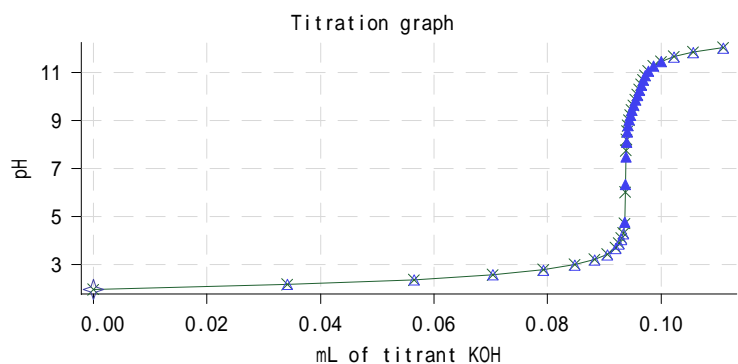
Sample

cs000256 concentration factor 0.842
 Base pKa 1 9.16

Sample graphs



Other graphs



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 Assay name: **pH-metric psKa**
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 Filename: **Y:\1108\11H-31007_cs000256_pH-metric psKa.t3r**

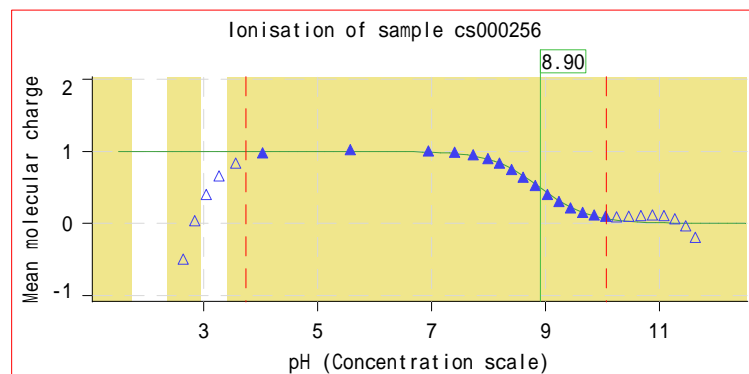
Experiment start time: **2011-8-31 13:03:34**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 311H-31007 Points 37 to 71

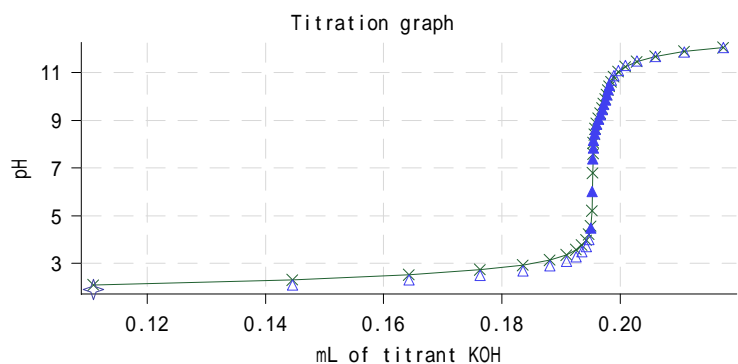
Sample

cs000256 concentration factor 0.832
 Base pKa 1 8.90

Sample graphs



Other graphs



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Experiment start time: **2011-8-31 13:03:34**

Assay name: **pH-metric psKa**

Analyst:

Assay ID: **11H-31007**

Instrument ID:


T311042

Filename: **Y:\1108\11H-31007_cs000256_pH-metric psKa.t3r**

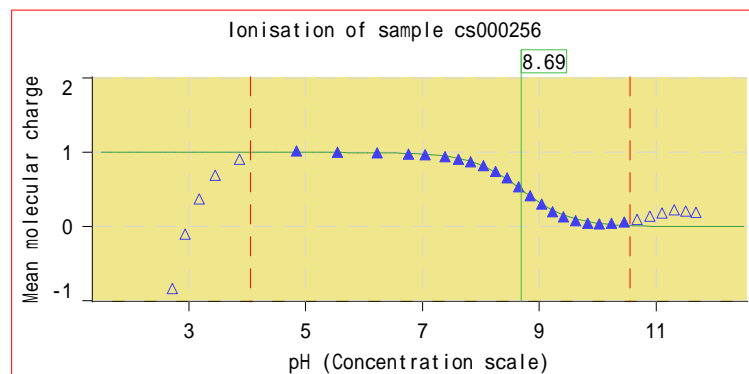
pH-metric psKa Titration 3 of 311H-31007 Points 72 to 109

Sample

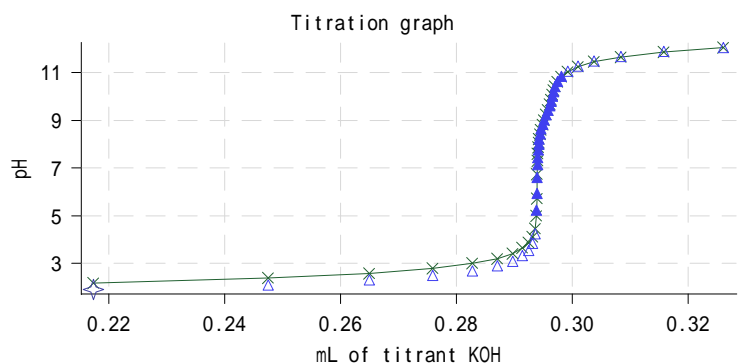
 cs000256 concentration factor 0.823

 Base pKa 1 8.69

Sample graphs



Other graphs





Assay model

Sample name: **cs000256**
Assay name: **pH-metric psKa**
Assay ID: **11H-31007**
Filename: **Y:\1108\11H-31007_cs000256_pH-metric psKa.t3r**

Experiment start time: **2011-8-31 13:03:34**
Analyst:
Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000256		
Sample by	Weight	2011-8-31 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample weight	0.000780 g		
Formula weight	503.35 g/mol		
Solubility	Unknown	2011-8-31 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	503.35		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	2011-8-31 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	8.00		
logp (XH +)	-10.00	2011-8-31 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		
