



## Yasuda-Shedlovsky Result

Sample name: **CS000252**  
Assay name: **pH-metric psKa**  
Assay ID: **11I-01019**  
Filename: **E:\T3 DATA\1109\11I-01019\_CS000252\_pH-metric psKa.t3r**

Experiment start time: **01/09/2011 17:29:07**  
Analyst:  
Instrument ID: **T311042**

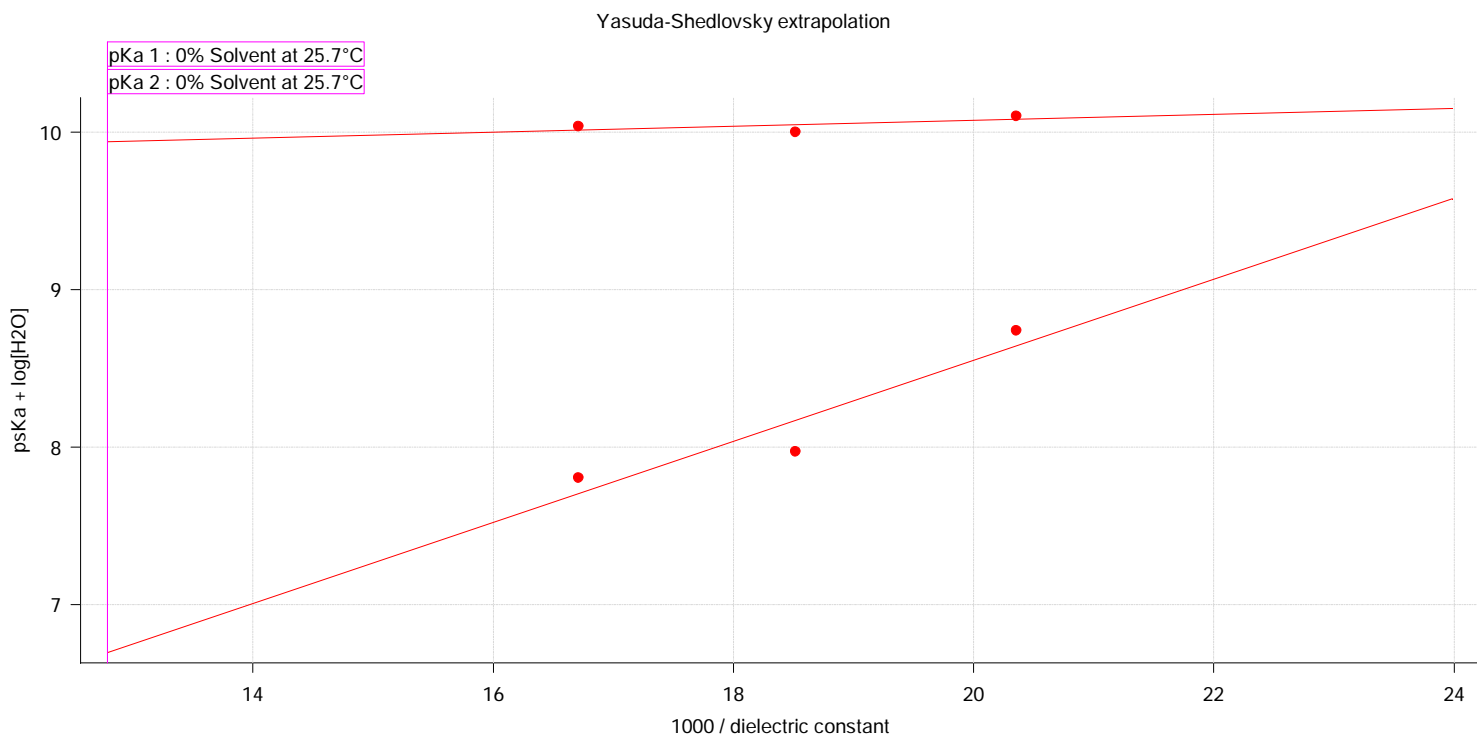
### Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	4.96	±0.56	3.42	256.7580	0.8797	0.170 M	25.7°C
Yasuda-Shedlovsky	8.19	±0.13	9.70	18.6997	0.4355	0.170 M	25.7°C

### Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H <sub>2</sub> O]	Ionic strength	Temperature	psKa 1	sK
11I-01019 Points 93 to 144	41.49 %	Up	pH-metric	59.8	29.1 M	0.175 M	26.4°C	✓	6.34 ✓ 1.57
11I-01019 Points 46 to 92	54.37 %	Up	pH-metric	54.0	22.0 M	0.171 M	26.0°C	✓	6.63 ✓ 1.61
11I-01019 Points 3 to 45	65.33 %	Up	pH-metric	49.1	16.3 M	0.163 M	24.8°C	✓	7.53 ✓ 1.81

### Graphs



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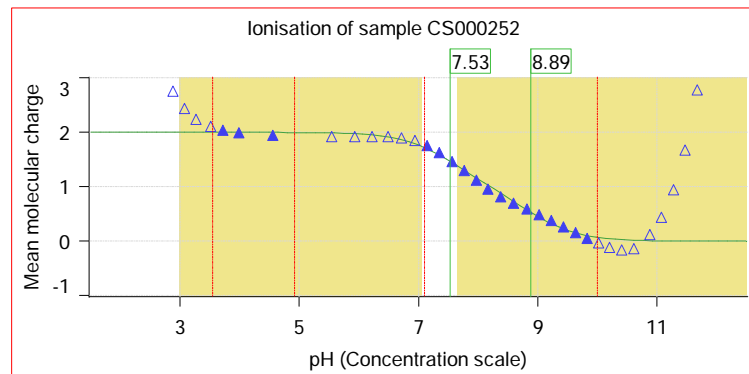
Experiment start time: **01/09/2011 17:29:07**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 1 of 3 11I-01019 Points 3 to 45

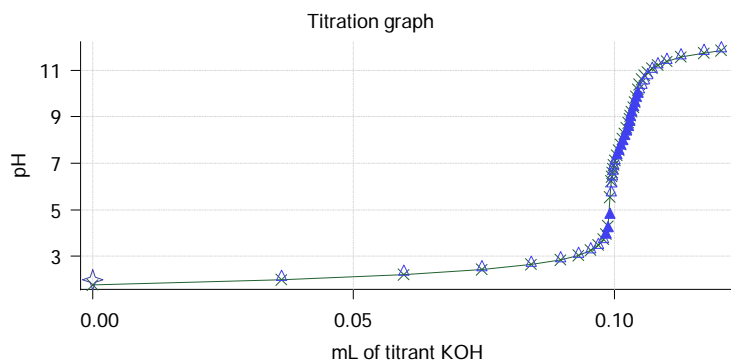
### Sample

CS000252 concentration factor 0.400  
 Base pKa 1 7.53  
 Base pKa 2 8.89

### Sample graphs



### Other graphs



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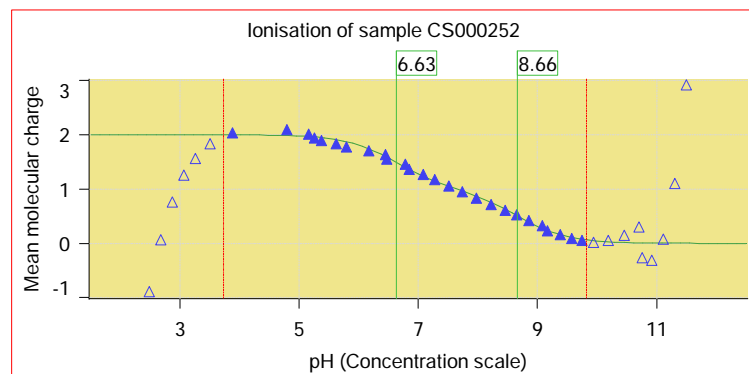
Experiment start time: **01/09/2011 17:29:07**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 2 of 3 11I-01019 Points 46 to 92

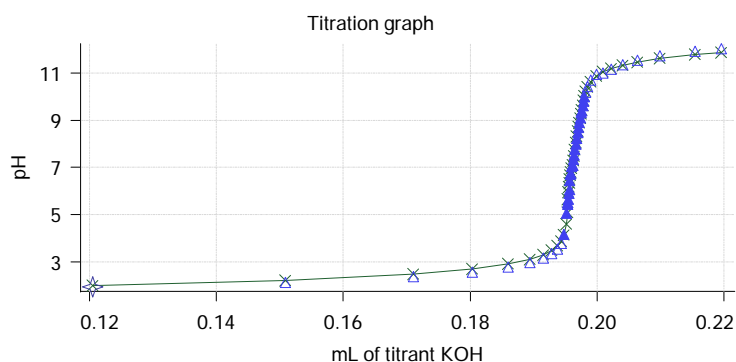
### Sample

CS000252 concentration factor 0.241  
 Base pKa 1 6.63  
 Base pKa 2 8.66

### Sample graphs



### Other graphs



Sample name: **CS000252**  
 Assay name: **pH-metric psKa**  
 Assay ID: **11I-01019**  
 Filename: **E:\T3 DATA\1109\11I-01019\_CS000252\_pH-metric psKa.t3r**

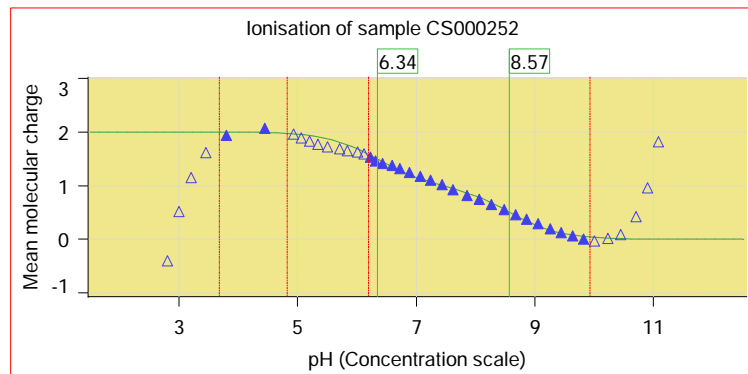
Experiment start time: **01/09/2011 17:29:07**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 3 of 3 11I-01019 Points 93 to 144

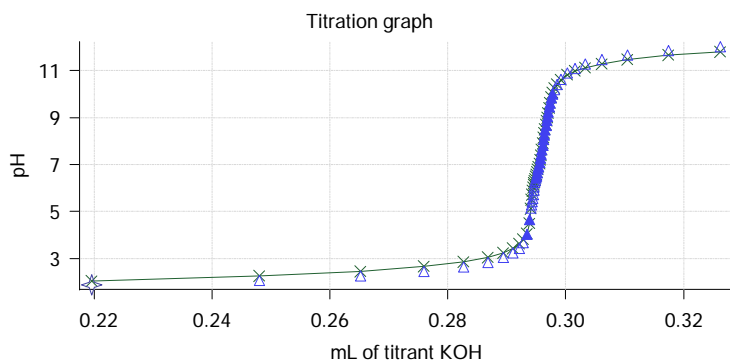
### Sample

CS000252 concentration factor 0.247  
 Base pKa 1 6.34  
 Base pKa 2 8.57

### Sample graphs



### Other graphs



### Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000252		
Sample by	Weight		
Sample weight	0.000900 g		
Formula weight	347.37 g/mol		
Solubility	Unknown	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	347.37		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	7.00		
pKa 2	8.00		
logP (XH2 2+)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00		
logP (neutral X)	-10.00		