



## Yasuda-Shedlovsky Result

Sample name: **CS000204**  
Assay name: **pH-metric psKa**  
Assay ID: **11I-16006**  
Filename: **E:\T3 DATA\1109\11I-16006\_CS000204\_pH-metric psKa.t3r**

Experiment start time: **16/09/2011 11:01:19**  
Analyst:  
Instrument ID: **T311042**

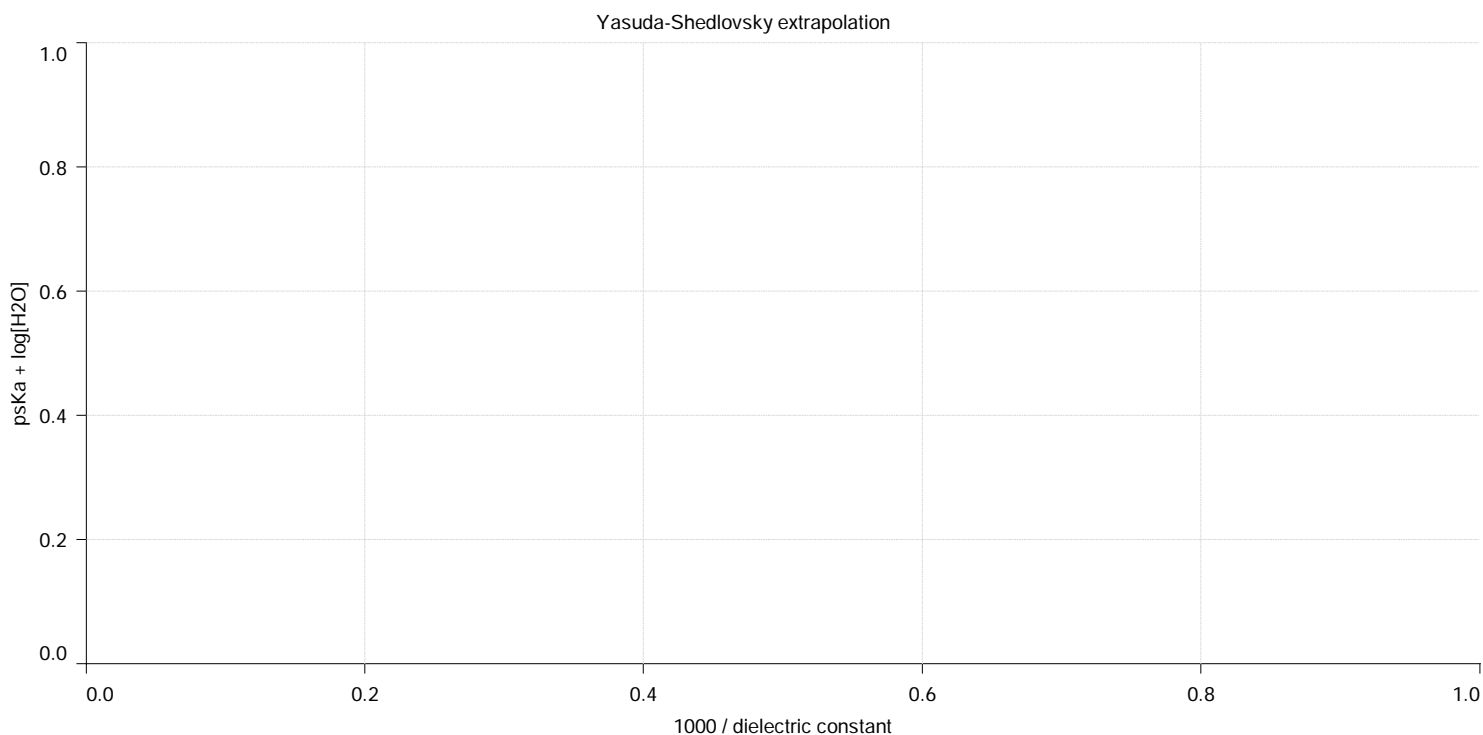
### Yasuda-Shedlovsky result

Extrapolation type pKa 0% SD Intercept Slope R<sup>2</sup> Ionic strength Temperature

### Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H <sub>2</sub> O]	Ionic strength	Temperature
11I-16006 Points 53 to 77	39.38 %	Up	pH-metric	60.8	30.3 M	0.179 M	26.4°C
11I-16006 Points 27 to 52	51.59 %	Up	pH-metric	55.6	23.5 M	0.173 M	25.1°C
11I-16006 Points 3 to 26	65.06 %	Up	pH-metric	49.5	16.5 M	0.162 M	23.8°C

### Graphs



Sample name: **CS000204**  
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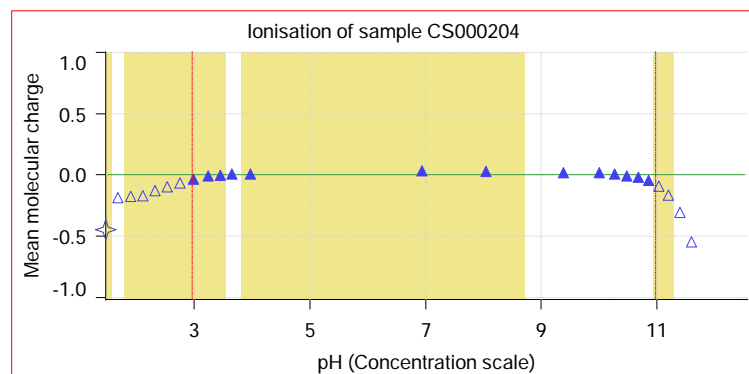
Experiment start time: **16/09/2011 11:01:19**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 1 of 3 11I-16006 Points 3 to 26

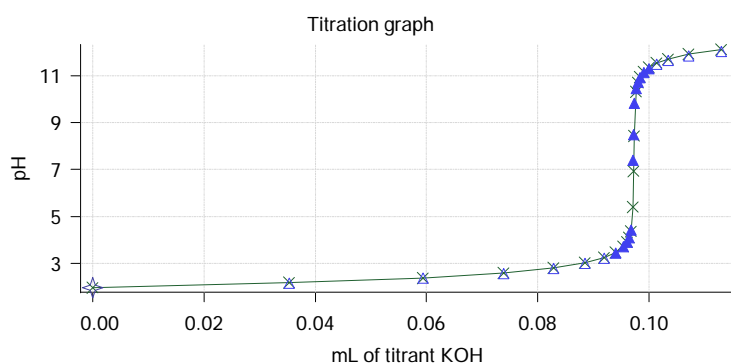
### Sample

 CS000204 concentration factor 0.885

### Sample graphs



### Other graphs



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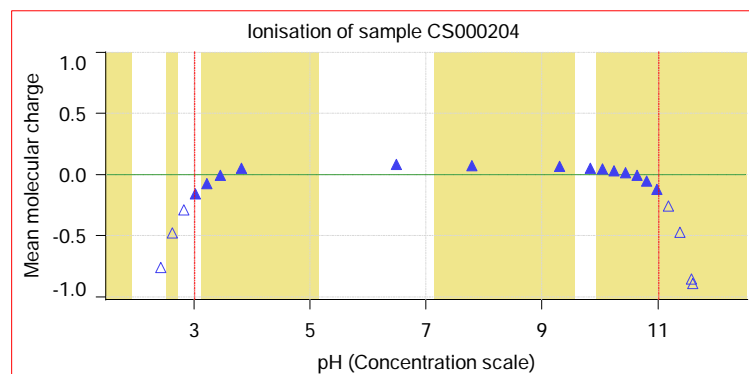
Experiment start time: **16/09/2011 11:01:19**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 2 of 3 11I-16006 Points 27 to 52

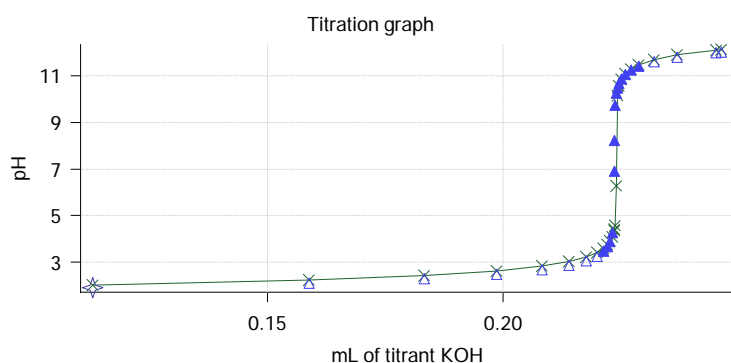
### Sample

 CS000204 concentration factor 1.009

### Sample graphs



### Other graphs



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 Assay ID: **11I-16006**  
 Filename: **E:\T3 DATA\1109\11I-16006\_CS000204\_pH-metric psKa.t3r**

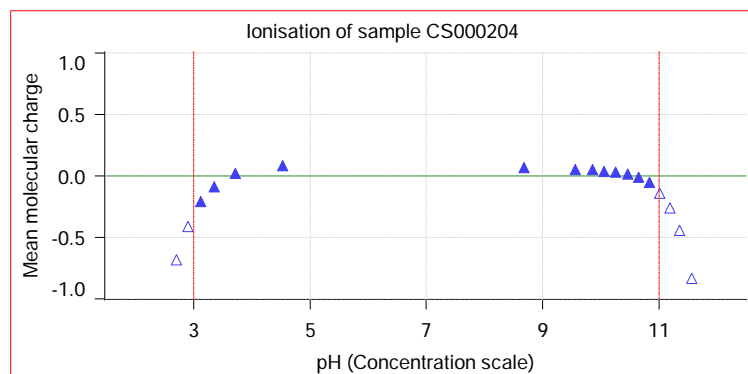
Experiment start time: **16/09/2011 11:01:19**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 3 of 3 11I-16006 Points 53 to 77

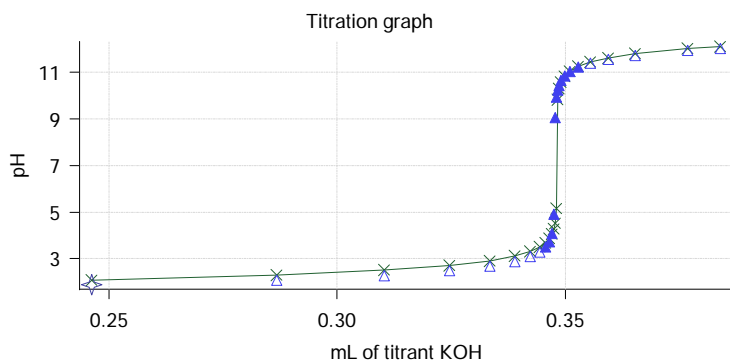
### Sample

 CS000204 concentration factor 1.030

### Sample graphs



### Other graphs



### Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000204		
Sample by	Weight		
Sample weight	0.001000 g		
Formula weight	349.34 g/mol		
Solubility	Unknown	16/09/2011 10:01:49	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	349.34		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00	16/09/2011 10:01:49	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r