

Représentation 3D du pH

Cas d'un acide en fonction d'un ajout de base et d'une dilution globale : cf. [cet article](#)

```
<sxh python; title : pH-3D_topo-01.py> #!/usr/bin/env python # -*- coding: utf-8 -*- """ Use of
numpy polynomes to compute pH of weak acid and strong base
```

3D topographic surface generation in the same conditions as the following paper : 3-D Surface Visualization of pH Titration “Topos”: Equivalence Point Cliffs, Dilution Ramps, and Buffer Plateaus” Garon C. Smith, Md Mainul Hossain and Patrick MacCarthy J. Chem. Educ., 2014, 91 (2), pp 225–231 DOI: 10.1021/ed400297t see fig here : <http://pubs.acs.org/doi/abs/10.1021/ed400297t>

Python code under GPLv3 GNU General Public License <http://www.gnu.org/licenses/gpl-3.0.html>

```
Didier Villers, UMONS http://dvillers.umons.ac.be/blog/contact/ """ import numpy as np import
numpy.polynomial.polynomial as poly import matplotlib.pyplot as plt from mpl_toolkits.mplot3d
import * # Axes3D from matplotlib import cm # Colors
```

```
def pH_monoprotic_acid(log10dil,Vb):
```

```
    # this Python function operate on numbers and cannot be applied on
    ndarrays due to the polynomial roots search
    dil=10**log10dil
    Ca=Ca0*dil
    Cb=Cb0*dil
    #
    http://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.polynomial.polyroots.html#numpy.polynomial.polynomial.polyroots
    #
    http://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.polynomial.polyval.html#numpy.polynomial.polynomial.polyval
    p=np.array([-Ka*Kw, -Kw-Ka*(Ca*Va-Cb*Vb)/(Va+Vb),Ka+(Cb*Vb)/(Va+Vb),1])
    x=poly.polyroots(p)
    return float(-np.log10(x[np.where(abs(x-27.5)<27.5)])) # only significant
    [H+] is returned
```

```
Ka=1.75E-5 # acid constant (acetic acid) Kw=1.E-14 # water product Ca0=1. # acid concentration
Cb0=1. # base concentration Va=0.1 # volume of acid Vb=0. # volume of added base log10dil=0
print(pH_monoprotic_acid(log10dil,Vb)) # sample call
```

```
fig = plt.figure() ax = Axes3D(fig) X,Y = np.linspace(-9.,0.,36), np.linspace(0.,200.,21) print(type(X),
X.ndim, X.shape, X.dtype) print(type(Y), Y.ndim, Y.shape, Y.dtype) Xc, Yc = np.meshgrid(X, Y) Z =
Xc+Yc # just to create Z print(type(Xc), Xc.ndim, Xc.shape, Xc.dtype) print(type(Yc), Yc.ndim,
Yc.shape, Yc.dtype) print(type(Z), Z.ndim, Z.shape, Z.dtype) print(range(len(X))) for ix in
range(len(X)):
```

```
    for iy in range(len(Y)):
        # print ix, iy,X[ix],Y[iy],pH_monoprotic_acid(X[ix],1E-3*Y[iy])
        Z[iy][ix] = pH_monoprotic_acid(X[ix],1E-3*Y[iy])
```

```
ax.plot_surface(Xc,Yc,Z, rstride=1,cstride=1,cmap=cm.jet) ax.set_xlabel('Log of dilution')  
ax.set_ylabel('Vb') ax.set_zlabel('pH') plt.show() </sxh>
```

La figure obtenue avec la librairie 3D de Matplotlib peut être manipulée (zoom, rotations). En voici une image correspondant à la figure de l'article référencé dans Journal of Chemical Education :



Prolongements, références

- [3-D Topo Surface Visualization of Acid-Base Species Distributions: Corner Buttes, Corner Pits, Curving Ridge Crests, and Dilution Plains](#) Garon C. Smith and Md Mainul Hossain, J. Chem. Educ., 2017, 94 (5), pp 598-605 DOI: 10.1021/acs.jchemed.6b00682

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