

Pythonによる化学シミュレーション入門

第6回 演習問題解答例

演習6・1, 6・2

```
import numpy as np
import matplotlib.pyplot as plt
from toeq import euler

kf, kb, tmax, h, a0, b0 = 2.0, 1.0, 3.0, 0.01, 1, 0
tt, aa, bb = euler(kf, kb, tmax, h, a0, b0)
plt.plot(tt, aa, label=f'[A] $k_f$ = {kf}, $k_b$ = {kb} ')
plt.plot(tt, bb, label='[B]')

print(f'kf/kb = {kf/kb}')
print(f'K = {bb[-1]/aa[-1]}')

kf, kb, tmax, h, a0, b0 = 1.0, 2.5, 3.0, 0.01, 1, 0
tt, aa, bb = euler(kf, kb, tmax, h, a0, b0)
plt.plot(tt, aa, '--', label=f'[A] $k_f$ = {kf}, $k_b$ = {kb} ')
plt.plot(tt, bb, '--', label='[B]')

print(f'kf/kb = {kf/kb}')
print(f'K = {bb[-1]/aa[-1]}')

plt.xlabel('Time')
plt.ylabel('Concentration')
plt.legend()
plt.show()
```

演習6・3

```
import numpy as np
import matplotlib.pyplot as plt
from toeq import euler

kf, kb, tmax, h, a0, b0 = 2.0, 1.0, 3.0, 0.01, 1, 0
tt, aa, bb = euler(kf, kb, tmax, h, a0, b0)
plt.plot(tt, aa, label=f'[A] $k_f$ = {kf}, $k_b$ = {kb} ')
plt.plot(tt, bb, label='[B]')

a8 = kb*a0/(kf+kb)
ax = (a0-a8)*np.exp(-(kf+kb)*tt) + a8
bx = a0 - ax
plt.plot(tt, ax, '--', label='[A] exact')
plt.plot(tt, bx, '--', label='[B] exact')

kf, kb, tmax, h, a0, b0 = 1.0, 2.5, 3.0, 0.01, 1, 0
tt, aa, bb = euler(kf, kb, tmax, h, a0, b0)
plt.plot(tt, aa, label=f'[A] $k_f$ = {kf}, $k_b$ = {kb} ')
plt.plot(tt, bb, label='[B]')
```

```

a8 = kb*a0/(kf+kb)
ax = (a0-a8)*np.exp(-(kf+kb)*tt) + a8
bx = a0 - ax
plt.plot(tt, ax, '--', label='[A] exact')
plt.plot(tt, bx, '--', label='[B] exact')

plt.xlabel('Time')
plt.ylabel('Concentration')
plt.legend()
plt.show()

```

演習6・4

```

import numpy as np
import matplotlib.pyplot as plt
from preeq import euler

kf, kb, kr, tmax, h, a0, b0, c0 = 2.0, 1.0, 0.3, 8.0, 0.01, 1, 0, 0
tt, aa, bb, cc = euler(kf, kb, kr, tmax, h, a0, b0, c0)
plt.plot(tt, aa, label=f'[A] $k_f$={kf}, $k_b$={kb}, $k_r$={kr} ')
plt.plot(tt, bb, label='[B]')
plt.plot(tt, cc, label='[C]')

plt.xlabel('Time')
plt.ylabel('Concentration')
plt.legend()
plt.show()

plt.plot(tt, bb/aa, label='[B]/[A]')
plt.xlabel('Time')
plt.ylabel('[B]/[A]')
plt.legend()
plt.show()

```