

1. (40 pts)

To solve this problem, use a spreadsheet or computer program, gather constants (in cgs units) and needed formulas:

Gas constant: $R=8.314 \times 10^7$

Temperature in Kelvin (20C): $T=293.15$

Viscosity of solvent (Water at 20C): $\eta=0.01$

Density of solvent (Water at 20C): $\rho=1.0$

Avogadro's number: $N=6.02214 \times 10^{23}$

$s = 4.2 \times 10^{-13}$ sec

$D = 7.5 \times 10^{-7}$ cm²/sec

PSV = 0.72 ml/g (and .55 ml/g)

Formulas, used in this order:

$$\begin{array}{llllll} f = \frac{RT}{ND} & M = \frac{sRT}{D(1-\bar{v}\rho)} & R_s = \frac{f}{6\pi\eta} & V_0 = \frac{M\bar{v}}{N} & r_0 = \left(\frac{3V_0}{4\pi}\right)^{1/3} & f_0 = 6\pi\eta r_0 \\ \text{Eq. 1} & \text{Eq. 2} & \text{Eq. 3} & \text{Eq. 4} & \text{Eq. 5} & \text{Eq. 6} \end{array}$$

Frictional Ratio: f/f_0

Output of program or spreadsheet:

C++ program example:

```
#include <iostream>
```

```
#include <math.h>
```

```
#include <vector>
```

```
using namespace std;
```

```
int main (int argc, char *argv[])
```

```
{
```

```
// Declare variables, stick to cgs units for everything:
```

```
// s (in sec), D (in cm2/sec), rho (density, in g/cm3)
```

```
// eta (viscosity, in g/(cm*sec)), R (gas constant, in erg/(K*Mol))
```

```
// T (temperature, in Kelvin), M (molar mass, in g/Mol)
```

```
// vbar (partial specific volume, in cm3/g), f (frictional coefficient, in g/sec)
```

```
// f0 (frictional coefficient of minimal sphere)
```

```
// ff0 (frictional ratio, dimensionless)
```

```
// r (radius of molecule, in cm), r0 (radius of minimal sphere, in cm)
```

```
// rs (radius of Stokes Sphere, in cm), V0 (volume of minimal sphere, in cm3)
```

```
// Assign constants:
```

```
double s=4.2e-13, D=7.5e-7, rho=1.0, R=8.314e7, T=293.15,
```

```
M,vbar=0.72, Avogadro=6.0221408e+23, eta=0.01; // eta has units of poise, or g/(cm*sec)
```

```
// Declare variables:
```

```
double f, f0, ff0, r, r0, V, V0, Vdiff, rs;
```

```
// calculate frictional coefficient (in g/sec, or cm*poise, poise units: g/(cm*sec)):
```

```
f = R*T/(D*Avogadro);
```

```
// Calculate Stokes Radius (in cm):
```

```

rs = f/(6*M_PI*eta);
// Calculate molar mass (in Dalton, or grams/mol):
M=s*R*T/(D*(1-vbar*rho));
// Calculate volume of minimal sphere (in cm^3, or ml):
V0 = M*vbar/Avogadro;
// Calculate radius of minimal sphere (in cm):
r0 = pow(V0*3.0/(4.0*M_PI), 1.0/3.0);
// Calculate frictional coefficient of minimal sphere (in cm*poise):
f0 = 6.0*M_PI*eta*r0;
// Calculate frictional ratio (dimensionless):
ff0 = f/f0;
// Output result:
cout << "V0: " << V0 << " cm^3\nrs: " << rs << " cm\nr0: "
<< r0 << " cm\nf: " << f << " g/sec\nf0: " << f0
<< " g/sec\nM: " << M
<< " Dalton\nf/f0: " << ff0 << endl;
}

```

(copy and paste into a file called ‘prog.cpp’ and compile with: ‘g++ prog.cpp’ on Linux)

Problem 1

Output with $vbar=0.72$ ml/g:

V0: 5.82789e-20 cm³
rs: 2.86277e-07 cm
r0: 2.40514e-07 cm
f: 5.3962e-08 g/sec
f0: 4.53359e-08 g/sec
M: 48745 Dalton
f/f0: 1.19027

Problem 2

Output with $vbar=0.55$ ml/g:

V0: 2.77005e-20 cm³
rs: 2.86277e-07 cm
r0: 1.87701e-07 cm
f: 5.3962e-08 g/sec
f0: 3.53808e-08 g/sec
M: 30330.2 Dalton
f/f0: 1.52518

Values **listed in red** change when the partial specific volume is changed. Try to explain *why* these values change.

3. (12 pts)

a. a molecule changes conformation and unfolds from globular to extended.

s and D decrease, because the friction and the frictional ratio increase when the molecule becomes more elongated. D and s are both inversely proportional to the frictional coefficient. The molar mass stays the same.

b) the density of the solvent increases

s decreases, because the buoyancy $(1 - vbar * rho)$ changes as the solvent density increases. D stays the same, because D is not dependent on the density of the solvent. The friction and frictional ratio also don't change, because they are not affected by the density of the solvent. The molar mass stays the same.

c) the viscosity of the solvent decreases

If the viscosity decreases, the molecule has less friction and s and D both increase, because both are inversely proportional to the friction. The frictional ratio however does not change, since the shape of the molecule is not changing, and neither does the molar mass.