Describes the partitioning of isotopes between two phases, A and B, produced by equilibrium or kinetic processes or some combination.

Typically, $\alpha \sim 1.001$ to $1.040$ except for D/H in certain cases.

Sometimes used: $\varepsilon = 1000(\alpha - 1)$

Confusion with different epsilon units used in Nd isotope studies
Isotope Ratio: \( R = \frac{D}{H} \quad ^{13}C/^ {12}C \quad ^{18}O/^ {16}O \quad etc. \)

\[
\delta = 1000 \left( \frac{R_x - R_{std}}{R_{std}} \right)
\]

\[
\alpha_{A-B} = \frac{R_A}{R_B}
\]

Relation between \( \alpha \) and \( \delta \)?
Isotope Ratio: $R = \frac{D}{H}, \frac{^{13}C}{^{12}C}, \frac{^{18}O}{^{16}O}, \text{etc.}$

$$\delta = 1000 \frac{R_x - R_{std}}{R_{std}}$$

$$\alpha_{A-B} = \frac{R_A}{R_B} = \frac{1000 + \delta A}{1000 + \delta B}$$
Relation between $\alpha$ and $\delta$

$$\alpha_{A-B} = \frac{1000 + \delta_A}{1000 + \delta_B}$$

*where* $\delta_A$ and $\delta_B$ must be reported relative to the same isotopic standard

**Important & exact relation**

Use to calculate the apparent or measured fractionation factor from the $\delta$-values of two associated phases

Use to predict the $\delta$-value of one phase from that of another if the fractionation factor $\alpha$ is known.
"BIG DELTA"

\[ \Delta \equiv \delta_A - \delta_B \]

Big Delta provides a convenient but rough estimate of the "fractionation" between the two phases.

e.g. \[
\begin{align*}
\delta_A &= +15.0\text{‰} \\
\delta_B &= -5.0\text{‰} \\
\Delta_{A-B} &= 20.0\text{‰}
\end{align*}
\]

A geochemist would state that "there is a 20 per mil fractionation between phases A and B", but the actual value of \( \alpha_{A-B} \) would be close to 1.0201
Exact

\[ \alpha_{_{A-B}} = \frac{1000 + \delta_A}{1000 + \delta_B} \]

\[ \alpha - 1 = \frac{1000 + \delta_A}{1000 + \delta_B} - \frac{1000 + \delta_B}{1000 + \delta_B} = \frac{\delta_A - \delta_B}{1000 + \delta_B} \]

Approximations

\[ 1000(\alpha - 1) \cong \delta_A - \delta_B \]

\[ 1000 \ln \alpha \cong \delta_A - \delta_B \]

\[ \Delta_{_{A-B}} \equiv \delta_A - \delta_B \cong 1000 \ln \alpha \cong 1000(\alpha - 1) \]
STANDARD CONVERSION IDENTITY

It is commonly necessary to convert the δ-value of a sample ("X") measured relative to one isotopic standard ("S1") to that which would be measured relative to another ("S2").

This conversion is approximately made by adding the per mil difference, $\delta_{S2S1}$ between the two standards, but for an exact conversion use:

$$\delta_{S2}X = \delta_{S1}X + \delta_{S2S1} + \frac{1}{1000}(\delta_{S1}X)(\delta_{S2S1})$$

e.g.

$$\left( \delta^{18}O_x \right)_{SMOW} = 1.03086 \left( \delta^{18}O_x \right)_{PDB} + 30.86$$
after Friedman & O’Neil (1977)
Bob Method for STANDARD CONVERSION

\[ \beta = \frac{1000 + \delta X_{\text{Std1}}}{1000 + \delta X_{\text{Std2}}} \]

where

\[ \beta = \frac{R_{\text{Std1}}}{R_{\text{Std2}}} \]

\( e.g. \)

\[ 1.03086 = \frac{1000 + \delta X_{\text{SMOW}}}{1000 + \delta X_{\text{PDB}}} \]
Material Balance Relationships

Bulk isotope ratio of a multi-component system:

\[ R_{\text{system}} = \frac{\sum_{j=1}^{n} N_j^*}{\sum_{j=1}^{n} N_j} \]
\[
R_{\text{system}} = \frac{\sum_{j=1}^{n} N_j^*}{\sum_{j=1}^{n} N_j} = \frac{N_1^* + N_2^* + \ldots + N_n^*}{\sum_{j=1}^{n} N_j}
\]

\[
R_{\text{system}} = \frac{N_1}{\sum_{j=1}^{n} N_j} \left( \frac{N_1^*}{N_1} \right) + \frac{N_2}{\sum_{j=1}^{n} N_j} \left( \frac{N_2^*}{N_2} \right) + \ldots
\]

\[
R_{\text{system}} = \sum_{j=1}^{n} X_j R_j
\]

where the \( X_i \) are the mole fractions of the reference nuclide of interest, such that:

\[
\sum_{j=1}^{n} X_j = 1
\]
Simple Binary Mixing

\[
\frac{(R_1 + R_2)}{2}
\]
For a trace isotope of a minor element, the mole fractions $X_i$ are:

$$X_k = \frac{C_k M_k}{\sum_{j=1}^{n} C_j M_j}$$

For binary mixing:

$$\left[ \frac{C_B}{C_A} \left( \frac{R^\dagger_{Mix} - R^\dagger_B}{R^\dagger_{Mix} - R^\dagger_A} \right) \right]_{Element L} = \left[ \frac{C_B}{C_A} \left( \frac{R^\dagger_{Mix} - R^\dagger_B}{R^\dagger_{Mix} - R^\dagger_A} \right) \right]_{Element M} = \ldots = -\frac{\text{Mass } A}{\text{Mass } B}$$

where

$$R^\dagger = \frac{\text{Mass of Isotope}}{\text{Total Mass of Element}}$$

Very nearly,

$R^\dagger \Rightarrow R$ substitution is OK for the H, C and O isotopic systems.
Ch 2 Probs 1, 3, 5, 7, 9, 10
ISOTOPIC EXCHANGE REACTIONS & CLASSICAL THERMODYNAMICS

Isotopic Exchange Reactions

\[ a \text{AM}^*_{b} + c \text{BM}_d = a \text{AM}_b + c \text{BM}^*_d \]

No. of atoms exchanged = \( a \times b = c \times d \)

Exchange reaction between homogeneous molecules:

\( \text{H}_2\text{O} + \text{D}_2 = \text{D}_2\text{O} + \text{H}_2 \)

Exchange of homogeneous and heterogeneous molecules:

\( \text{H}_2\text{O} + \text{HD} = \text{HDO} + \text{H}_2 \)

\[ K = \frac{[\text{HDO}][\text{H}_2]}{[\text{H}_2\text{O}][\text{HD}]} = 3.7 \text{ @ } 25^\circ\text{C} \]
1) How large are $K$’s for isotopic exchange reactions?

2) Can ordinary thermodynamic relationships be used to evaluate $K$?

3) What does $R$ relate to the thermodynamic activities of the isotopic species?

4) What is the relationship between $K$ and $\alpha$?

5) How do $\alpha$ and $K$ depend on $T$ and $P$?
Classical Thermodynamics

Reaction Isotherm

\[ \Delta G^\circ = -RT \ln K \]

van’t Hoff eq.

\[ \frac{\partial \ln K}{\partial T} = \frac{\Delta H_{rxn}^\circ}{RT^2} \]

integrate

\[ \ln K = - \frac{\Delta H_{rxn}^\circ}{RT} + \text{const} \]

Clausius-Clapeyron eq.

\[ \ln \frac{P}{P_0} = - \frac{\Delta H_{rxn}^\circ}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right) \]
Example Calculation:

Find the equilibrium constant for D/H exchange between hydrogen gas and liquid water

\[ \text{H}_2\text{O}_{\text{liq}} + \text{HD}_{\text{gas}} = \text{HDO}_{\text{liq}} + \text{H}_2 \text{ gas} \]
<table>
<thead>
<tr>
<th>SUBSTANCE</th>
<th>$\Delta H_f^\circ$ kcal/mole</th>
<th>$S^\circ$ cal/mole-deg</th>
<th>$\Delta G_f^\circ$ kcal/mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$ (g)</td>
<td>0.00</td>
<td>31.208</td>
<td>0.00</td>
</tr>
<tr>
<td>HD (g)</td>
<td>0.076</td>
<td>34.343</td>
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</table>
Example Calculation:

\[
\begin{align*}
\text{H}_2\text{O}_{\text{liq}} + \text{HD}_{\text{gas}} &= \text{HDO}_{\text{liq}} + \text{H}_2 \text{ gas} \\
\text{-56687} &\quad \text{-350} \quad \text{-57817} \quad \text{0.00} \\
\Delta G^\circ_{\text{rxn}} &= \text{-780 cal/mole} \\
\text{=>} \quad K &= 3.73
\end{align*}
\]
Example Calculation #2:

\[
\text{H}_2\text{O}_{\text{liq}} + \text{HDO}_{\text{gas}} = \text{HDO}_{\text{liq}} + \text{H}_2\text{O}_{\text{gas}}
\]

\[
-56687 \quad -55719 \quad -57817 \quad -54634
\]

\[\Delta G_{\text{rxn}}^\circ = -45 \text{ cal/mole}\]

\[\Rightarrow K = 1.079\]

*Small difference: significant figures*
<table>
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</table>
Example Calculation #3:

Vapor Pressure @ 25°C:

\[ \begin{align*}
\text{H}_2\text{O}_{\text{liq}} &= \text{H}_2\text{O}_{\text{vapor}} \\
\Delta G^\circ_{\text{rxn}} &= +2053 \text{ cal/mole} \\
\Rightarrow P^\circ_{\text{H}_2\text{O}} &= 0.03126 \text{ atm} \\
&= 23.76 \text{ torr}
\end{align*} \]
### Example Calculations:

**Vapor Pressures @ 25°C:**

\[
\begin{align*}
\text{H}_2\text{O}_{\text{liq}} &= \text{H}_2\text{O}_{\text{vapor}} & \Delta G^\circ_{\text{rxn}} &= 2053 \text{ cal/mole} \quad \Rightarrow P^\circ_{\text{H}_2\text{O}} &= 23.76 \text{ torr} \\
\text{HDO}_{\text{liq}} &= \text{HDO}_{\text{vapor}} & \Delta G^\circ_{\text{rxn}} &= 2098 \text{ cal/mole} \quad \Rightarrow P^\circ_{\text{HDO}} &= 22.02 \text{ torr} \\
\text{D}_2\text{O}_{\text{liq}} &= \text{D}_2\text{O}_{\text{vapor}} & \Delta G^\circ_{\text{rxn}} &= 2136 \text{ cal/mole} \quad \Rightarrow P^\circ_{\text{D}_2\text{O}} &= 20.65 \text{ torr}
\end{align*}
\]

\[
P^\circ_{\text{H}_2\text{O}} / P^\circ_{\text{HDO}} = 1.079
\]

\[
P^\circ_{\text{H}_2\text{O}} / P^\circ_{\text{D}_2\text{O}} = 1.151
\]

\[
\text{SQRT} \left( P^\circ_{\text{H}_2\text{O}} / P^\circ_{\text{D}_2\text{O}} \right) = 1.073 \quad \text{rule of the mean}
\]
**Symmetry Numbers**
Number of indistinguishable ways that a given molecule can be oriented in space.

Heteronuclear diatomic molecules: \( \sigma = 1 \)  
HF  \ CO  \ \overset{16}{O}^{18}O

Homonuclear diatomic molecules: \( \sigma = 2 \)  
H\(_2\)  \ \overset{16}{O}^{16}O

Methane  
\( \sigma = 12 \)  \ CH\(_4\)
**Symmetry Numbers**
Number of indistinguishable ways that a given molecule can be oriented in space.

<table>
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<td>$\sigma=2$</td>
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<td>Methane</td>
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Two isotopes, M and M*, with relative abundances of x & y

\[ x + y = 1 \]

Overall isotope ratio: \( R = y/x \)

If isotopes are randomly distributed among s identical sites: binomial expansion

\[(x + y)^s = x^s + sx^{s-1}y + (s/2)(s-1)x^{s-2}y^2 + \ldots + y^s\]

Normalized activity of any species is given by the appropriate term of the expansion

or

\[ a_{M_{s-r}M^*_r} = \frac{s!}{(s-r)! \ r!} \ x^{s-r} \ y^r \]

\[ s = \# \text{ sites} \]
Relationship between Species Activities and Isotope Ratios

Two isotopes, M and M*, with relative abundances of x & y

\[ x + y = 1 \]

Overall isotope ratio: \( R = \frac{y}{x} \)

If isotopes are randomly distributed among s identical sites: binomial expansion

\[ (x + y)^s = x^s + s x^{s-1} y + (s/2) (s-1) x^{s-2} y^2 + \ldots + y^s \]

Normalized activity of any species is given by the appropriate term of the expansion.

Criss’ relationship between R and activity ratio, \( a^*/a \), of two isotopologues

\[ R = \left( \frac{a^* \sigma^*}{a \sigma} \right)^{1/b} \]

where \( b = r_1 - r_2 \)

r = # rare atoms

b is the difference between the # of sites occupied by the heavy isotope in the two isotopologues.

Complications arise for molecules having distinguishable varieties for single isotopic compositions; i.e., where the distribution of isotopes among the sites is not random
- e.g. left and right-handed varieties
- e.g. trans and cis forms of a square planar molecule.
- e.g. different isomeric forms have different energies
Three isotopes: abundances $x$, $y$ and $z$ in a molecule with $s$ sites:

$$1 = (x + y + z)^s$$

Number of distinguishable isotologues relating to the distribution of $p$ isotopes among $s$ identical sites is given by the combinatorial equation:

$$\# \text{ Species} = \frac{(p + s - 1)!}{(p - 1)! \, s!}$$

e.g. $O_2 \Rightarrow 6$
Statistical Thermodynamics

Total # of particles N in the system:
\[ N = \sum_{i} n_i \]

Total internal energy of the system:
\[ E = \sum_{i} n_i \varepsilon_i \]

Boltzmann distribution law:
The fraction or probability \( P_i \) of molecules with energy \( \varepsilon_i \) decreases exponentially with the magnitude of that energy level:
\[
P_i = \frac{n_i}{N} = \frac{g_i e^{-\varepsilon_i/kT}}{\sum_i g_i e^{-\varepsilon_i/kT}}
\]

Average Energy
\[
\overline{E} = \frac{\sum_{n=1}^{\infty} n_i \varepsilon_i}{N} = \sum_{n=1}^{\infty} P_i \varepsilon_i
\]

Partition Coefficient
\[
Q = \sum_i g_i e^{-\varepsilon_i/kT}
\]
Relation of \( Q \) to thermodynamic Quantities

\[
Q = \sum_i g_i e^{-\varepsilon_i / kT}
\]

\[
\bar{E} = kT^2 \left( \frac{\partial \ln Q}{\partial T} \right)_{N,V}
\]

\[
A = -kT \ln Q
\]

\[
E_{total} = E_1 + E_2 + E_3 + ... + E_n
\]

\[
Q_{total} = Q_1 Q_2 Q_3 ... Q_n
\]

Isotopic Exchange Reaction:

\[
a \text{AM}^*_b + c \text{BM}_d = a \text{AM}_b + c \text{BM}^*_d
\]

\[
K = \frac{\left( \frac{Q_{BM}^*}{Q_{BM}_d} \right)^c \left( \frac{Q_{AM}}{Q_{AM}_b} \right)^a}{\left( \frac{Q_{BM}_d}{Q_{BM}^*} \right)^c \left( \frac{Q_{AM}_b}{Q_{AM}^*} \right)^a}
\]
\[ Q = \sum_{i} g_i e^{-\varepsilon_i / kT} \]

**Isotopic Exchange Reaction**

\[ a \ AM^*_b + c \ BM_d = a \ AM_b + c \ BM^*_d \]

No. of atoms exchanged \(= a \times b = c \times d\)

\[ K = \left( \frac{Q_{BM_d^*}}{Q_{BM_d}} \right)^c \left( \frac{Q_{AM_b^*}}{Q_{AM_b}} \right)^a = \left( \frac{Q_{BM_d^*}}{Q_{BM_d}} \right)^c \left( \frac{Q_{AM_b^*}}{Q_{AM_b}} \right)^a \]

\[ \alpha = \left( \frac{K}{K_\infty} \right)^{1/ac} \]

where

\[ K_\infty = \left( \frac{\sigma_{AM_b^*} / \sigma_{AM_b}}{\sigma_{BM_d^*} / \sigma_{BM_d}} \right)^c \]
Example

\[ 2 \text{H}_2^{18}\text{O} + \text{C}^{(16}\text{O})_2 = 2 \text{H}_2^{16}\text{O} + \text{C}^{(18}\text{O})_2 \]

\[ K = \frac{\left[ \frac{\text{H}_2^{16}\text{O}}{\text{H}_2^{18}\text{O}} \right]^2 \left[ \frac{\text{C}^{18}\text{O}_2}{\text{C}^{16}\text{O}_2} \right]}{\left[ \frac{\text{H}_2^{16}\text{O}}{\text{H}_2^{18}\text{O}} \right]^2 \left[ \frac{\text{C}^{18}\text{O}_2}{\text{C}^{16}\text{O}_2} \right]} \]

\[ \alpha = \]

\[ K_\infty = \]
Example

\[ 2 \text{H}_2^{18}\text{O} + \text{C}^{(16}\text{O})_2 = 2 \text{H}_2^{16}\text{O} + \text{C}^{(18}\text{O})_2 \]

\[ K = \frac{\left[ \text{H}_2^{16}\text{O} \right]^2 \left[ \text{C}^{18}\text{O}_2 \right]}{\left[ \text{H}_2^{18}\text{O} \right]^2 \left[ \text{C}^{16}\text{O}_2 \right]} \]

\[ \alpha = \frac{R_{\text{CO}_2}}{R_{\text{H}_2\text{O}}} = \frac{\left( \frac{^{18}\text{O}/^{16}\text{O}}{^{18}\text{O}/^{16}\text{O}} \right)_{\text{CO}_2}}{\left( \frac{^{18}\text{O}/^{16}\text{O}}{^{18}\text{O}/^{16}\text{O}} \right)_{\text{H}_2\text{O}}} \]

\[ K_\infty = \frac{\left( \sigma_{\text{H}_2^{18}\text{O}} \right)^2 \left( \sigma_{\text{C}^{18}\text{O}_2} \right)}{\left( \sigma_{\text{H}_2^{16}\text{O}} \right)^2 \left( \sigma_{\text{C}^{16}\text{O}_2} \right)} = \frac{2^2 \times 2}{2^2 \times 2} = 1 \]
Let $^{18}\text{O in CO}_2 = y$
& $^{16}\text{O in CO}_2 = x$

$[C^{18}\text{O}^{18}\text{O}] = y^2$
$[C^{16}\text{O}^{16}\text{O}] = x^2$
$[C^{18}\text{O}^{16}\text{O}] = 2xy$

$\left( \frac{^{18}\text{O}}{^{16}\text{O}} \right)_{\text{CO}_2} = \frac{2[C^{18}\text{O}^{18}\text{O}] + [C^{16}\text{O}^{18}\text{O}]}{2[C^{16}\text{O}^{16}\text{O}] + [C^{16}\text{O}^{18}\text{O}]} = \frac{2y^2 + 2xy}{2x^2 + 2xy} = \frac{2y(y + x)}{2x(x + y)} = \frac{y}{x}$

$\left( \frac{^{18}\text{O}}{^{16}\text{O}} \right)_{\text{H}_2\text{O}} = \frac{[H_2^{18}\text{O}]}{[H_2^{16}\text{O}]} = \frac{f}{e}$

Now
\[ \alpha = \frac{R_{\text{CO}_2}}{R_{\text{H}_2\text{O}}} = \frac{\left( \frac{^{18}\text{O}}{^{16}\text{O}} \right)_{\text{CO}_2}}{\left( \frac{^{18}\text{O}}{^{16}\text{O}} \right)_{\text{H}_2\text{O}}} = \frac{y}{x} \frac{f}{e} \]
Let $^{18}\text{O} \text{ in } \text{CO}_2 = y$ 
& $^{16}\text{O} \text{ in } \text{CO}_2 = x$

Let $^{18}\text{O} \text{ in } \text{H}_2\text{O} = f$
& $^{16}\text{O} \text{ in } \text{H}_2\text{O} = e$

$[C^{18}\text{O}^{18}\text{O}] = y^2$
$[C^{16}\text{O}^{16}\text{O}] = x^2$
$[C^{18}\text{O}^{16}\text{O}] = 2xy$

$[H_2^{18}\text{O}] = f$
$[H_2^{16}\text{O}] = e$

\[ K = \frac{[H_2^{16}\text{O}]}{[H_2^{18}\text{O}]} \frac{[C^{18}\text{O}_2]}{[C^{16}\text{O}_2]} = \frac{e^2 y^2}{f^2 x^2} = \left(\frac{e}{f} \frac{y}{x}\right)^2 = \alpha^2 \]

$\alpha = \frac{R_{\text{CO}_2}}{R_{\text{H}_2\text{O}}} = \frac{\left(\frac{^{18}\text{O}}{^{16}\text{O}}\right)_{\text{CO}_2}}{\left(\frac{^{18}\text{O}}{^{16}\text{O}}\right)_{\text{H}_2\text{O}}} = \frac{y}{x} \frac{f}{e}$
Simple Harmonic Oscillator  

The chemical bond acts like an “ideal” spring, with force proportional to the displacement:

\[ F = -kx \]

Integrate to find the potential energy \( V \):

\[ V = \frac{kx^2}{2} \]

Diff. Eq:

\[ F = ma = m \frac{d^2x}{dt^2} = -kx \]

Solution

\[ x = A \cos \left( \frac{\sqrt{k}}{m} t \right) \]

Period & Frequency:

\[ T = 2\pi \sqrt{\frac{k}{m}} \quad \text{so} \quad \nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \]
\[ \nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \]

where \( \mu = \frac{m_1 m_2}{m_1 + m_2} \)

\[ \nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \]
Inter-relationships

\[
\frac{\nu_{1,2}}{\nu_{1,1}} = \sqrt{\frac{\mu_{1,1}}{\mu_{1,2}}}
\]

or

\[
\frac{\omega_{1,2}}{\omega_{1,1}} = \sqrt{\frac{\mu_{1,1}}{\mu_{1,2}}}
\]

where the wavenumbers:

\[
\omega = \nu / c
\]

\[
\nu_{1,2}, \omega_{1,2}, \text{ and } \mu_{1,2} = \frac{m_1 m_2}{m_1 + m_2}
\]

\[
\nu_{1,1}, \omega_{1,1}, \text{ and } \mu_{1,1} = \frac{m_1 m_1}{m_1 + m_1} = \frac{m_1}{2}
\]
Table 2.2: Spectroscopic Data of Some Diatomic Molecules

<table>
<thead>
<tr>
<th>GAS</th>
<th>µ (amu)</th>
<th>ωe (cm⁻¹)</th>
<th>ωeχe (cm⁻¹)</th>
<th>Be (cm⁻¹)</th>
<th>Do (cm⁻¹)</th>
<th>re (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>0.5039126</td>
<td>4401.213</td>
<td>121.336</td>
<td>60.853</td>
<td>36118.26</td>
<td>0.74144</td>
</tr>
<tr>
<td>HD</td>
<td>0.6717113</td>
<td>3813.15</td>
<td>91.65</td>
<td>45.655</td>
<td>36406.20</td>
<td>0.74142</td>
</tr>
<tr>
<td>D₂</td>
<td>1.0070511</td>
<td>3115.50</td>
<td>61.82</td>
<td>30.4436</td>
<td>36748.91</td>
<td>0.74152</td>
</tr>
<tr>
<td>HF</td>
<td>0.9570554</td>
<td>4138.32</td>
<td>89.88</td>
<td>20.9557</td>
<td>47336.30</td>
<td>0.91680</td>
</tr>
<tr>
<td>DF</td>
<td>1.8210454</td>
<td>2998.192</td>
<td>45.761</td>
<td>11.0102</td>
<td>47892.82</td>
<td>0.91694</td>
</tr>
<tr>
<td>H³⁵Cl</td>
<td>0.9795927</td>
<td>2990.9463</td>
<td>52.8186</td>
<td>10.5934</td>
<td>35759.11</td>
<td>1.27455</td>
</tr>
<tr>
<td>D³⁵Cl</td>
<td>1.9044136</td>
<td>2145.163</td>
<td>27.1825</td>
<td>5.448794</td>
<td>36175.29</td>
<td>1.27458</td>
</tr>
<tr>
<td>^{16}O₂</td>
<td>7.9974575</td>
<td>1580.193</td>
<td>11.981</td>
<td>1.44563</td>
<td>41259.77</td>
<td>1.20752</td>
</tr>
</tbody>
</table>

Source: Huber and Herzberg (1979)
Simple Harmonic Oscillator (SHO)

\[
\nu_2 = \sqrt{\frac{\mu_1}{\mu_2}} \quad \omega_2 = \sqrt{\frac{\mu_1}{\mu_2}}
\]

where wavenumbers \( \omega = \frac{\nu}{c} \)

Energy Levels of SHO (Quantum mechanics)

\[
\varepsilon_{SHO} = \left( n + \frac{1}{2} \right) h \nu
\]

\( \varepsilon = \) vibrational energy
\( n = \) energy level \( 0, 1, 2, 3, \ldots \)
\( h = \) Planck’s constant
The graph represents a potential energy function $V(x)$ for a system involving the first several quantum states labeled by $n=0, 1, 2, 3, 4, 5, 6$. The label $n=0$ corresponds to the zero-point energy (ZPE). The potential energy is symmetric about the origin, with each level $n$ corresponding to an energy level that increases with $n$. The function is labeled as SHO (Simple Harmonic Oscillator).
End