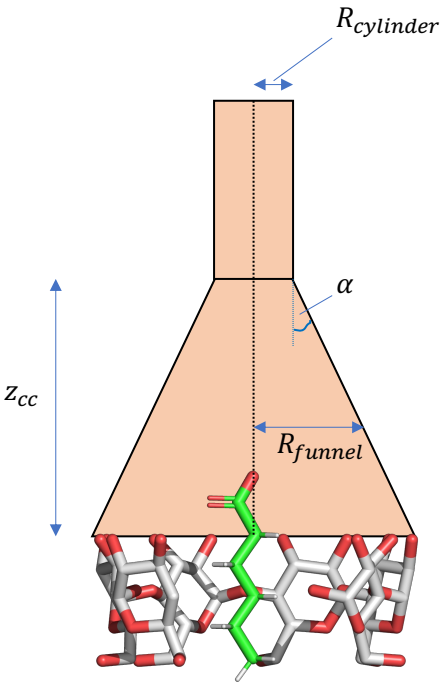
# Funnel Potential




- Reaction coordinate is the difference in center of mass (COM) between the guest and host molecule.
- Below I separated the $z$ and the $x$-$y$ plane. The $r_z$ will be used for the biasing with umbrella sampling (or metadynamics) and $r_{xy}$ will be used to apply the funnel potential

$$r_z = \vec{r}_{\mathrm{com}}(\mathrm{guest})_z - \vec{r}_{\mathrm{com}}(\mathrm{host})_z$$

$$r_{xy} = \vec{r}_{\mathrm{com}}(\mathrm{guest})_{xy} - \vec{r}_{\mathrm{com}}(\mathrm{host})_{xy}$$

- User specified parameters for the funnel potential
  - $\alpha$
  - $z_{cc}$
  - $k_{wall}$
  - $R_{cylinder}$

- Boundary of funnel at a given location on $z$

$$R_{funnel}(r_z) = (z_{cc} - |r_z|)\times\tan\alpha + R_{cylinder}$$

- Flat-bottom potential when guest is $\mathrm{r}_z \leq z_{cc}$, i.e., inside the funnel section

$$U_{funnel} = \frac{1}{2}k_{wall}\left(r_{xy} - R_{funnel}\right)^2$$

- Flat-bottom potential when guest is $\mathrm{r}_z > z_{cc}$, i.e., inside the cylinder section

$$U_{cylinder} = \frac{1}{2}k_{wall}\left(r_{xy} - R_{cylinder}\right)^2$$

- Flat-bottom potential of the whole "funnel"

$$U_{wall}(r_z) = \begin{cases} U_{funnel}(r_z) & \text{if } r_z \leq z_{cc} \\ U_{cyclinder}(r_z) & \text{otherwise} \end{cases}$$