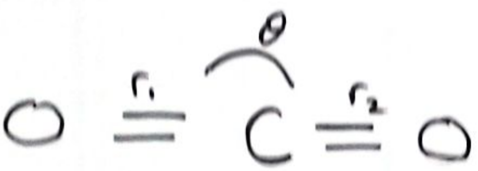
He

O = C = O

asymm. stret. CO_2



Symmetric stretch: $V(r) = MLR$

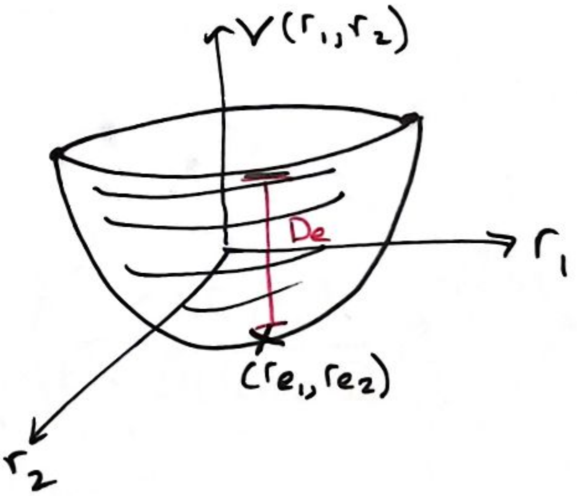
For each θ, $V_\theta(r) = MLR$.

① $V(r_1, r_2) = \xi\, D_e\left(1 - \frac{u(r_1, r_2)}{u(r_{e_1}, r_{e_2})} e^{-\beta(r_1, r_2)\, y_p(r_1, r_2)}\right)^2$

③ $r_1 \to \infty,\ \beta \to \beta_{\infty,1}$, $\quad (r_1, r_2) \to \infty,\ \beta_{\infty,1} + \beta_{\infty,2} = \beta_\infty$
$r_2 \to \infty,\ \beta \to \beta_{\infty,2}$

② $$\beta(r_1, r_2) = \sum_i \beta_i\, y_{p,1}(r_1)^{i} (1 - y_{p,1}) + y_{p,1}\beta_{\infty,1} + \sum_j \beta_j\, y_{p,2}(r_2)^{j} (1 - y_{p,2}) + y_{p,2}\beta_{\infty,2}$$

$V(r_{e_1}, r_{e_2})$



⑫ $$V_{LR}(r_1, r_2) = D_e(r_1, r_2) - \frac{C_{6,1}(r_2)}{r_1^6} - \frac{C_{8,1}(r_2)}{r_1^8} - \frac{C_{6,2}(r_1)}{r_2^6} - \frac{C_{8,2}(r_1)}{r_2^8}$$

$V_{LR}(r_1, r_2) = D_e - u(r_1, r_2)$

(4)
$$y_P = y_{P,1} \times y_{P,2}$$
$$y_P = \left(\frac{r_1^P - r_{e,1}^P}{r_1^P + r_{e,1}^P}\right)\left(\frac{r_2^P - r_{e,2}^P}{r_2^P + r_{e,2}^P}\right)$$

(5) $r_1 \to \infty \ , \quad y_P \to y_{P,2}$

(6) $\beta(r_1, r_2)\, y_P(r_1, r_2) \longrightarrow \beta_{\infty,1} + \beta(r_2)$

(7)
$$e^{-\beta_{\infty,1} - \beta(r_2) y_{P,2}}$$

(8)
$$e^{\overline{-\beta_{\infty,1}}} \, e^{-\beta(r_2) y_{P,2}}$$

(9)
$$V(r_1, r_2) \xrightarrow{r_1 \to \infty} \left\{ D_e \left(1 - \frac{u(r_1, r_2)}{u(r_{e,1}, r_{e_2})} e^{-\beta_{\infty,1}} e^{-\beta(r_2) y_{P,2}}\right)^2\right.$$

$$\cancel{\beta_{\infty,1} = \ln\left(\frac{u(r_e)}{4 D_e}\right)}$$

(10)
$$\beta_{\infty,1} = \ln\left(\frac{2 D_e}{u(r_{e,1})}\right)$$

$$V(r_1, r_2) \xrightarrow{r_1 \to \infty} \left\{ D_e \left(1 - \frac{u(r_1, r_2)}{\cancel{u(r_{e_1})}\, u(r_{e_2})} \frac{\cancel{u(r_{e_1})}}{2 D_e} e^{-\beta(r_2) y_{P,2}}\right)^2\right.$$

$$V(r_1,r_2) \xrightarrow{r_1 \to \infty} \left\{ D_e\left(1 - \frac{u(r_1,r_2)}{u(r_{e_2})2D_e}\, e^{-\beta(r_2)y_{p,2}}\right)^2 \right.$$

11

$$u(r_1,r_2) = \frac{C_{6,1}(r_2,\theta)}{r_1^6} + \frac{C_{8,1}(r_2,\theta)}{r_1^8} + \frac{C_{6,2}(r_1,\theta)}{r_2^6} + \frac{C_{8,2}(r_1,\theta)}{r_2^8}$$

in terms of r_1, 11 is just:

$$\left\{ D_e\left(1 - u(r_1,r_2) \times C\right)^2 \right.$$

①* $$V(r_1, r_2) = De\left(1 - \frac{u(r_1)}{u(r_{e,1})} e^{-\beta_1(r_1) y_{p,1}} - \underbrace{\frac{u(r_2)}{u(r_{e,2})} e^{-\beta_2(r_2) y_{p,2}}}_{M(R(r_2)) = M(r_2)}\right)^2$$

$r_1 \to \infty$

$$De\left(1 - \frac{u(r_1)}{u(r_{e,1})} e^{-\beta_{\infty,1}} - \frac{u(r_2)}{u(r_{e,2})} e^{-\beta_2(r_2) y_{p,2}}\right)^2$$

$$De\left(1 - \frac{u(r_1)}{u(r_{e,1})} e^{-\beta_1(r_1) y_{p,1}} - M(r_2)\right)^2$$

$$De - M(r_2) - u(r_1) + \frac{u(r_1)^2}{4(De - M(r_2))}$$

$r_2 \to \infty$

$$De\left(1 - \frac{u(r_2)}{u(r_{e,2})} e^{-\beta_2(r_2) y_{p,2}} - M(r_1)\right)^2$$

$$De - M(r_1) - u(r_2) + \frac{u(r_2)^2}{4(De - M(r_1))}$$

$r_1, r_2 \to \infty$:

$$De\left(1 - \frac{u(r_1)}{u(r_{e,1})} e^{-\beta_{1,\infty}} - \frac{u(r_2)}{u(r_{e,2})} e^{-\beta_{2,\infty}}\right)^2$$

$$\beta_{1,\infty}^{(r_2)} = \ln\left(\frac{2(De - M(r_2))}{u(r_{e,1})}\right)$$

$$\beta_{2,\infty}^{(r_1)} = \ln\left(\frac{2(De - M(r_1))}{u(r_{e,2})}\right)$$

$r_1 \to \infty$

$$De - 2De\frac{u(r_1)}{u(r_{e1})}e^{-\beta_{\infty,1}} - 2De\frac{u(r_2)}{u(r_{e2})}e^{-\cancel{\beta_2(r_2)}\,\cancel{y_{p_2}}^{1}\,\beta_{\infty_2}}$$

$$+ 2\frac{u(r_1)u(r_2)}{u(r_{e1})u(r_{e2})}e^{-\beta_{\infty,1}}e^{-\cancel{\beta_2(r_2)}^{\beta_{\infty_2}}\cancel{y_{p_2}}^{1}}$$

$$+ \frac{u(r_1)^2}{u(r_{e1})^2}e^{-2\beta_{\infty,1}} + \frac{u(r_2)^2}{u(r_{e2})^2}e^{-2\beta_2(r_2)\cancel{y_{p_2}}^{1}}$$

$r_1, r_2 \to \infty$:

$$De - 2\frac{De\,u(r_1)}{u(r_{e,1})}e^{-\beta_{\infty,1}} - 2\frac{De\,u(r_2)}{u(r_{e_2})}e^{-\beta_{\infty_2}}$$

$$+ 2\frac{u(r_1)u(r_2)}{u(r_{e,1})u(r_{e_2})}e^{-\beta_{\infty_1}}e^{-\beta_{\infty_2}}$$

$$+ \frac{u(r_1)^2}{u(r_{e,1})^2}e^{-2\beta_{\infty,1}} + \frac{u(r_2)^2}{u(r_{e,2})}e^{-2\beta_{\infty,2}}$$

$C_6 \equiv C_6(\cancel{r}, \theta_1, \theta_2)$ ~~C_6~~

$C_6 \equiv C_6(r_1, r_2, \theta)$

$$\frac{C_{6,1}(r_2, \theta)}{r_1^6}$$

C_6C

$C_6^8 \equiv \langle 0| C_6(\theta) |0\rangle$

$\underline{C_{6_1}} = \underline{C_{6_2}}, \; r_2 \to \infty, \; r_1 \to \infty.$

$C_{6,1}$