

## LAMPIRAN



## LAMPIRAN A

### HASIL PERHITUNGAN TEORI HMO UNTUK MOLEKUL FENOLFTALEIN DENGAN $k_{co} = 0.9$ DAN $h = 2$

#### A.1. Fenolftalein pada suasana asam

Perhitungan untuk mendapatkan panjang gelombang maksimum ( $\Delta E = E_{LUMO} - E_{HOMO}$ )

##### a.1. $\lambda$ maksimum kromofor I & II fenolftalein

$$\left[ \begin{array}{ccccccc|c} x+2 & 0.9 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.9 & x & 1 & 0 & 0 & 0 & 1 & \\ 0 & 1 & x & 1 & 0 & 0 & 0 & \\ 0 & 0 & 1 & x & 1 & 0 & 0 & \\ 0 & 0 & 0 & 1 & x & 1 & 0 & \\ 0 & 0 & 0 & 0 & 1 & x & 1 & \\ 0 & 1 & 0 & 0 & 0 & 1 & x & \end{array} \right] \xrightarrow{\text{solve}, x \rightarrow} \left[ \begin{array}{c} 1 \\ -1 \\ -2.6944640949536582796 \\ -1.6003167254356062814 \\ -0.8448343063285823526 \\ 1.0518727015330546489 \\ 2.0877424251847922646 \end{array} \right]$$

$$(-.745 - 1) - 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{\frac{6.626 \cdot 10^{-34} \cdot J \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}}}{\lambda} \quad \text{solve, } \lambda \rightarrow 217.684738 \text{ nm}$$

#### a.2. Fungsi gelombang kromofor I & II fenolftalein

$$\psi_1 = 0.788\phi_1 + 0.480\phi_2 + 0.232\phi_3 + 0.126\phi_4 + 0.097\phi_5 + 0.126\phi_6 + 0.232\phi_7$$

$$\psi_2 = 0.113\phi_1 + 0.458\phi_2 + 0.412\phi_3 + 0.385\phi_4 + 0.376\phi_5 + 0.385\phi_6 + 0.412\phi_7$$

$$\psi_3 = 0.431\phi_1 + 0.090\phi_2 + 0.297\phi_3 + 0.440\phi_4 + 0.492\phi_5 + 0.440\phi_6 + 0.297\phi_7$$

$$\psi_4 = 0\phi_1 + 0\phi_2 - 0.500\phi_3 - 0.500\phi_4 + 0\phi_5 + 0.500\phi_6 + 0.500\phi_7$$

$$\psi_5 = 0.384\phi_1 - 0.477\phi_2 - 0.372\phi_3 + 0.197\phi_4 + 0.520\phi_5 + 0.197\phi_6 - 0.372\phi_7$$

$$\psi_6 = 0\phi_1 + 0\phi_2 + 0.500\phi_3 - 0.500\phi_4 + 0\phi_5 + 0.500\phi_6 - 0.500\phi_7$$

$$\psi_7 = -0.183\phi_1 + 0.569\phi_2 - 0.224\phi_3 - 0.321\phi_4 + 0.580\phi_5 - 0.321\phi_6 - 0.224\phi_7$$

### a.3. Indeks kereaktifan

#### - Kerapatan elektron

$$q_1 = 2 \cdot (0.788)^2 + 2 \cdot (0.48)^2 + 2 \cdot (0.232)^2 + 2 \cdot (0.126)^2 \rightarrow q_1 = 1.842088$$

$$q_2 = 2 \cdot (0.113)^2 + 2 \cdot (0.458)^2 + 2 \cdot (0.412)^2 + 2 \cdot (0.385)^2 \rightarrow q_2 = 1.081004$$

$$q_3 = 2 \cdot (0.431)^2 + 2 \cdot (0.09)^2 + 2 \cdot (0.297)^2 + 2 \cdot (0.44)^2 \rightarrow q_3 = .95134$$

$$q_4 = 2 \cdot (0)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.5)^2 + 2 \cdot (-0.5)^2 \rightarrow q_4 = 1.0$$

$$q_5 = 2 \cdot (0.384)^2 + 2 \cdot (-0.477)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (0.197)^2 \rightarrow q_5 = 1.104356$$

$$q_6 = 2 \cdot (0)^2 + 2 \cdot (0)^2 + 2 \cdot (0.5)^2 + 2 \cdot (-0.5)^2 \rightarrow q_6 = 1.0$$

$$q_7 = 2 \cdot (-0.183)^2 + 2 \cdot (0.569)^2 + 2 \cdot (-0.274)^2 + 2 \cdot (-0.321)^2 \rightarrow q_7 = 1.070734$$

#### - Orde ikatan

$$P_{12} = 2 \cdot (0.788 \cdot 0.48) + 2 \cdot (0.113 \cdot 0.458) + 2 \cdot (0.431 \cdot 0.09) + 2 \cdot (0) \rightarrow P_{12} = .937568$$

$$P_{23} = 2 \cdot (0.232 \cdot 0.48) + 2 \cdot (0.412 \cdot 0.458) + 2 \cdot (0.297 \cdot 0.09) + 2 \cdot (0 \cdot -0.5) \rightarrow P_{23} = .653572$$

$$P_{27} = 2 \cdot (0.232 \cdot 0.48) + 2 \cdot (0.412 \cdot 0.458) + 2 \cdot (0.297 \cdot 0.09) + 2 \cdot (0 \cdot -0.5) \rightarrow P_{27} = .653572$$

$$P_{34} = 2 \cdot (0.232 \cdot 0.126) + 2 \cdot (0.412 \cdot 0.385) + 2 \cdot (0.297 \cdot 0.44) + 2 \cdot (-0.5 \cdot -0.5) \rightarrow P_{34} = 1.137064$$

$$P_{45} = 2 \cdot (0.097 \cdot 0.126) + 2 \cdot (0.376 \cdot 0.385) + 2 \cdot (0.492 \cdot 0.44) + 2 \cdot (0 \cdot -0.5) \rightarrow P_{45} = .746924$$

$$P_{56} = 2 \cdot (0.097 \cdot 0.126) + 2 \cdot (0.376 \cdot 0.385) + 2 \cdot (0.492 \cdot 0.44) + 2 \cdot (0 \cdot 0.5) \rightarrow P_{56} = .746924$$

$$P_{67} = 2 \cdot (0.232 \cdot 0.126) + 2 \cdot (0.412 \cdot 0.385) + 2 \cdot (0.297 \cdot 0.44) + 2 \cdot (0.5 \cdot 0.5) \rightarrow P_{67} = 1.137064$$

#### - Valensi bebas

$$F_1 = \sqrt{3 - .937568} \text{ solve } , F_1 \rightarrow .7944828075688772935$$

$$F_2 = \sqrt{3 - .937568 - 0.653572 - 0.653572} \text{ solve } , F_2 \rightarrow -.5126611924311227065$$

$$F_3 = \sqrt{3 - 0.653572 - 1.137064} \text{ solve } , F_3 \rightarrow -.058585192431122706500$$

$$F_4 = \sqrt{3 - .746924 - 1.137064} \text{ solve } , F_4 \rightarrow -.1519371924311227065$$

$$F_5 = \sqrt{3 - .746924 - .746924} \text{ solve } , F_5 \rightarrow .2382028075688772935$$

$$F_6 = \sqrt{3 - .746924 - 1.137064} \text{ solve } , F_6 \rightarrow -.1519371924311227065$$

$$F_7 = \sqrt{3 - .653572 - 1.137064} \text{ solve } , F_7 \rightarrow -.058585192431122706500$$

b.1.  $\lambda$  maksimum kromofor III fenolflalein

$$\left[ \begin{array}{ccccccc} x & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & x & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & x & 0.9 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.9 & x + 2 \end{array} \right] \xrightarrow{\text{solve, } x \rightarrow} \begin{array}{c} 1 \\ -1 \\ -2.6469845868146363748 \\ -1.8125324870039759652 \\ -1.1737583044947627072 \\ .59202222113183780315 \\ 1.2890562807039950215 \\ 2.1521968764775422225 \end{array}$$

$$(-1 - .59202) \cdot 75390 \cdot 4.18 \frac{J}{\text{mol}} = \frac{\frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}}}{\lambda} \xrightarrow{\text{solve, } \lambda \rightarrow 238.602 \cdot \text{nm}}$$

b.2. Fungsi gelombang kromofor III.

$$\psi_1 = 0.162 \downarrow_1 + 0.098 \downarrow_2 + 0.08 \downarrow_3 + 0.098 \downarrow_4 + 0.162 \downarrow_5 + 0.301 \downarrow_6 + 0.418 \downarrow_7 + 0.81 \downarrow_8$$

$$\psi_2 = -0.372 \downarrow_1 - 0.3725 \downarrow_2 - 0.372 \downarrow_3 - 0.372 \downarrow_4 - 0.372 \downarrow_5 - 0.372 \downarrow_6 - 0 \downarrow_7 + 0.413 \downarrow_8$$

$$\psi_3 = -0.403 \downarrow_1 + 0.345 \downarrow_2 - 0.327 \downarrow_3 + 0.345 \downarrow_4 - 0.403 \downarrow_5 + 0.506 \downarrow_6 - 0.264 \downarrow_7 + 0.058 \downarrow_8$$

$$\psi_4 = -0.083 \downarrow_1 - 0.358 \downarrow_2 + 0.55 \downarrow_3 - 0.358 \downarrow_4 - 0.083 \downarrow_5 + 0.467 \downarrow_6 - 0.441 \downarrow_7 + 0.12 \downarrow_8$$

$$\psi_5 = -0.354 \downarrow_1 - 0.038 \downarrow_2 + 0.372 \downarrow_3 - 0.038 \downarrow_4 - 0.364 \downarrow_5 + 0.114 \downarrow_6 + 0.705 \downarrow_7 - 0.269 \downarrow_8$$

$$\psi_6 = -0.183 \downarrow_1 + 0.321 \downarrow_2 + 0.555 \downarrow_3 + 0.321 \downarrow_4 - 0.183 \downarrow_5 - 0.533 \downarrow_6 - 0.251 \downarrow_7 + 0.269 \downarrow_8$$

$$\psi_7 = 0.5 \downarrow_1 - 0.5 \downarrow_2 - 0 \downarrow_3 + 0.5 \downarrow_4 - 0.5 \downarrow_5 - 0 \downarrow_6 - 0 \downarrow_7 + 0 \downarrow_8$$

$$\psi_8 = -0.5 \downarrow_1 + 0.5 \downarrow_2 + 0 \downarrow_3 - 0.5 \downarrow_4 - 0.5 \downarrow_5 + 0 \downarrow_6 + 0 \downarrow_7 + 0 \downarrow_8$$

### b.3. Indeks kereaktifan

#### - Kerapatan elektron

$$\begin{aligned}q_1 &= 2(0.162)^2 + 2(0.098)^2 + 2(0.08)^2 + 2(0.098)^2 \rightarrow q_1 = 1.03704 \\q_2 &= 2(-0.372)^2 + 2(-0.372)^2 + 2(-0.372)^2 + 2(-0.372)^2 \rightarrow q_2 = 1.107072 \\q_3 &= 2(-0.403)^2 + 2(0.345)^2 + 2(-0.327)^2 + 2(0.345)^2 \rightarrow q_3 = 1.014776 \\q_4 &= 2(-0.083)^2 + 2(-0.358)^2 + 2(0.55)^2 + 2(-0.358)^2 \rightarrow q_4 = 1.131434 \\q_5 &= 2(-0.364)^2 + 2(-0.038)^2 + 2(0.372)^2 + 2(-0.038)^2 \rightarrow q_5 = .547536 \\q_6 &= 2(-0.183)^2 + 2(0.321)^2 + 2(0.555)^2 + 2(0.321)^2 \rightarrow q_6 = 1.095192 \\q_7 &= 2(0.5)^2 + 2(-0.5)^2 + 2(0)^2 + 2(0.5)^2 \rightarrow q_7 = 1.5 \\q_8 &= 2(-0.5)^2 + 2(0.5)^2 + 2(0)^2 + 2(0.5)^2 \rightarrow q_8 = 1.5\end{aligned}$$

#### - Orde ikatan

$$\begin{aligned}P_{12} &= 2(0.162 \cdot 0.098) + 2(-0.372 \cdot -0.372) + 2(-0.403 \cdot 0.345) + 2(-0.083 \cdot -0.358) \rightarrow P_{12} = .089878 \\P_{16} &= 2(0.162 \cdot 0.301) + 2(-0.372 \cdot -0.372) + 2(-0.403 \cdot 0.506) + 2(-0.083 \cdot 0.467) \rightarrow P_{16} = -.111066 \\P_{23} &= 2(0.08 \cdot 0.098) + 2(-0.372 \cdot -0.372) + 2(-0.372 \cdot 0.345) + 2(-0.358 \cdot -0.358) \rightarrow P_{23} = .292096 \\P_{34} &= 2(0.08 \cdot 0.098) + 2(-0.372 \cdot -0.372) + 2(-0.372 \cdot 0.345) + 2(-0.358 \cdot -0.358) \rightarrow P_{34} = .292096 \\P_{45} &= 2(0.162 \cdot 0.098) + 2(-0.372 \cdot -0.372) + 2(-0.403 \cdot 0.345) + 2(-0.083 \cdot -0.358) \rightarrow P_{45} = .089878 \\P_{47} &= 2(0.418 \cdot 0.098) + 2(0 \cdot -0.372) + 2(-0.264 \cdot 0.345) + 2(-0.441 \cdot -0.358) \rightarrow P_{47} = .215524 \\P_{56} &= 2(0.162 \cdot 0.301) + 2(-0.372 \cdot -0.372) + 2(-0.403 \cdot 0.506) + 2(-0.083 \cdot 0.467) \rightarrow P_{56} = -.111066 \\P_{78} &= 2(0.418 \cdot 0.81) + 2(0 \cdot 0.413) + 2(-0.264 \cdot 0.058) + 2(-0.441 \cdot 0.12) \rightarrow P_{78} = .540696\end{aligned}$$

#### - Valensi bebas

$$\begin{aligned}F_1 &= \sqrt{3} - .089878 - -.111066 \text{ solve } F_1 \rightarrow 1.7532388075688772935 \\F_2 &= \sqrt{3} - .089878 - .292096 \text{ solve } F_2 \rightarrow 1.3500768075688772935 \\F_3 &= \sqrt{3} - .292096 - .292096 \text{ solve } F_3 \rightarrow 1.1478588075688772935 \\F_4 &= \sqrt{3} - .292096 - .089878 \text{ solve } F_4 \rightarrow 1.3500768075688772935 \\F_5 &= \sqrt{3} - -.111066 - .089878 \text{ solve } F_5 \rightarrow 1.7532388075688772935 \\F_6 &= \sqrt{3} - -.111066 - -.111066 \text{ solve } F_6 \rightarrow 1.9541828075688772935 \\F_7 &= \sqrt{3} - .215524 - .540696 \text{ solve } F_7 \rightarrow .9758308075688772935 \\F_8 &= \sqrt{3} - .540696 \text{ solve } F_8 \rightarrow 1.1913548075688772935\end{aligned}$$

## A.2. Fenolftalein dalam suasana basa ( kromofor I )

### a.1. $\lambda$ maksimum

$$\left[ \begin{array}{cccccccccccccc|c} x+2 & 0.9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.9 & x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 0.9 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x+2 \end{array} \right] \rightarrow \begin{array}{l} -3.6265906458769951894 \\ -2.1705686402092637527 \\ -2.1705686402092637527 \\ -1.6283791127181430161 \\ -1.2598105633758029294 \\ -1.2598105633758029294 \\ -.66226891904713808389 \\ -.15793840724625132514 \\ .37087716344618915957 \\ .66226891904713808389 \\ 1.0149808153902353822 \\ 1.0149808153902353822 \\ 1.2292924440286587586 \\ 1.6985296833538622835 \\ 1.6985296833538622835 \\ 2.514881053591343067 \end{array}$$

solve ,  $x \rightarrow$

$$\frac{6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{mol}} = \frac{\text{sec} \cdot \text{mol}}{\lambda}$$

solve ,  $x \rightarrow 718.32201715972590504 \text{ nm}$

### a.2. Fungsi gelombang

$$\begin{aligned} \psi_1 = & 0.063\phi_1 + 0.124\phi_2 + 0.181\phi_3 + 0.231\phi_4 + 0.274\phi_5 + 0.307\phi_6 + 0.330\phi_7 + 0.342\phi_8 \\ & + 0.342\phi_9 + 0.33\phi_{10} + 0.307\phi_{11} + 0.274\phi_{12} + 0.231\phi_{13} + 0.181\phi_{14} + 0.124\phi_{15} \\ & + 0.063\phi_{16} \end{aligned}$$

$$\begin{aligned} \psi_2 = & 0.124\phi_1 + 0.231\phi_2 + 0.307\phi_3 + 0.342\phi_4 + 0.330\phi_5 + 0.274\phi_6 + 0.181\phi_7 + 0.064\phi_8 \\ & + 0.062\phi_9 - 0.181\phi_{10} - 0.273\phi_{11} - 0.330\phi_{12} - 0.342\phi_{13} + 0.307\phi_{14} - 0.232\phi_{15} - \\ & 0.125\phi_{16} \end{aligned}$$

$$\begin{aligned} \psi_3 = & 0.182\phi_1 + 0.308\phi_2 + 0.341\phi_3 + 0.273\phi_4 + 0.123\phi_5 - 0.064\phi_6 - 0.231\phi_7 - 0.330\phi_8 - \\ & 0.330\phi_9 - 0.232\phi_{10} - 0.064\phi_{11} + 0.120\phi_{12} + 0.273\phi_{13} - 0.341\phi_{14} - 0.308\phi_{15} + \\ & 0.182\phi_{16} \end{aligned}$$

$$\psi_4 = 0.231\phi_1 + 0.342\phi_2 + 0.274\phi_3 + 0.064\phi_4 - 0.180\phi_5 - 0.330\phi_6 + 0.307\phi_7 - 0.125\phi_8 + 0.123\phi_9 + 0.306\phi_{10} + 0.330\phi_{11} + 0.182\phi_{12} - 0.061\phi_{13} + 0.273\phi_{14} - 0.342\phi_{15} - 0.233\phi_{16}$$

$$\psi_5 = 0.274\phi_1 + 0.330\phi_2 + 0.124\phi_3 - 0.180\phi_4 - 0.341\phi_5 - 0.232\phi_6 + 0.062\phi_7 + 0.306\phi_8 + 0.308\phi_9 + 0.065\phi_{10} - 0.230\phi_{11} - 0.342\phi_{12} - 0.182\phi_{13} + 0.122\phi_{14} + 0.329\phi_{15} + 0.275\phi_{16}$$

$$\psi_6 = 0.307\phi_1 + 0.274\phi_2 - 0.064\phi_3 - 0.330\phi_4 - 0.232\phi_5 + 0.123\phi_6 + 0.341\phi_7 + 0.182\phi_8 - 0.179\phi_9 - 0.342\phi_{10} - 0.126\phi_{11} + 0.229\phi_{12} + 0.331\phi_{13} + 0.066\phi_{14} - 0.272\phi_{15} - 0.308$$

$$\psi_7 = 0.330\phi_1 + 0.181\phi_2 + 0.231\phi_3 + 0.307\phi_4 + 0.062\phi_5 + 0.341\phi_6 + 0.125\phi_7 + 0.273\phi_8 - 0.275\phi_9 + 0.122\phi_{10} + 0.342\phi_{11} - 0.066\phi_{12} - 0.306\phi_{13} - 0.233\phi_{14} + 0.178\phi_{15} + 0.331\phi_{16}$$

$$\psi_8 = 0.342\phi_1 + 0.064\phi_2 - 0.330\phi_3 - 0.125\phi_4 + 0.308\phi_5 + 0.182\phi_6 + 0.273\phi_7 + 0.223\phi_8 + 0.229\phi_9 + 0.275\phi_{10} - 0.178\phi_{11} + 0.308\phi_{12} + 0.122\phi_{13} + 0.331\phi_{14} - 0.059\phi_{15} - 0.342\phi_{16}$$

$$\psi_9 = 0.342\phi_1 + 0.062\phi_2 - 0.330\phi_3 + 0.123\phi_4 + 0.308\phi_5 - 0.179\phi_6 + 0.275\phi_7 + 0.229\phi_8 + 0.233\phi_9 + 0.272\phi_{10} + 0.183\phi_{11} + 0.305\phi_{12} + 0.127\phi_{13} - 0.239\phi_{14} - 0.067\phi_{15} + 0.341\phi_{16}$$

$$\psi_{10} = 0.330\phi_1 - 0.180\phi_2 - 0.232\phi_3 + 0.306\phi_4 + 0.065\phi_5 - 0.342\phi_6 + 0.122\phi_7 - 0.275\phi_8 - 0.272\phi_9 - 0.27\phi_{10} + 0.341\phi_{11} - 0.059\phi_{12} - 0.309\phi_{13} + 0.228\phi_{14} + 0.185\phi_{15} - 0.238\phi_{16}$$

$$\psi_{11} = 0.274\phi_1 - 0.273\phi_2 - 0.064\phi_3 + 0.330\phi_4 - 0.230\phi_5 - 0.126\phi_6 + 0.342\phi_7 - 0.178\phi_8 - 0.183\phi_9 + 0.341\phi_{10} + 0.12\phi_{11} - 0.234\phi_{12} + 0.329\phi_{13} - 0.058\phi_{14} - 0.277\phi_{15} + 0.304\phi_{16}$$

$$\psi_{12} = 0.231\phi_1 - 0.330\phi_2 + 0.123\phi_3 + 0.182\phi_4 - 0.342\phi_5 + 0.229\phi_6 + 0.066\phi_7 + 0.308\phi_8 + 0.305\phi_9 - 0.059\phi_{10} - 0.234\phi_{11} + 0.341\phi_{12} - 0.176\phi_{13} - 0.129\phi_{14} + 0.331\phi_{15} - 0.270\phi_{16}$$

$$\psi_{13} = 0.231\phi_1 - 0.342\phi_2 + 0.273\phi_3 - 0.061\phi_4 - 0.182\phi_5 + 0.331\phi_6 - 0.306\phi_7 + 0.121\phi_8 + 0.127\phi_9 - 0.309\phi_{10} + 0.329\phi_{11} - 0.176\phi_{12} - 0.068\phi_{13} + 0.277\phi_{14} - 0.341\phi_{15} + 0.226\phi_{16}$$

$$\Psi_{14} = 0.182\phi_1 - 0.307\phi_2 + 0.341\phi_3 - 0.273\phi_4 + 0.122\phi_5 + 0.066\phi_6 - 0.233\phi_7 + 0.331\phi_8 - 0.329\phi_9 + 0.228\phi_{10} - 0.058\phi_{11} - 0.129\phi_{12} + 0.277\phi_{13} - 0.342\phi_{14} + 0.304\phi_{15} - 0.174\phi_{16}$$

$$\Psi_{15} = 0.124\phi_1 - 0.232\phi_2 + 0.308\phi_3 - 0.342\phi_4 + 0.329\phi_5 - 0.272\phi_6 + 0.178\phi_7 - 0.059\phi_8 - 0.067\phi_9 + 0.185\phi_{10} - 0.277\phi_{11} + 0.331\phi_{12} - 0.341\phi_{13} + 0.304\phi_{14} - 0.226\phi_{15} + 0.117\phi_{16}$$

$$\Psi_{16} = 0.063\phi_1 - 0.125\phi_2 + 0.182\phi_3 - 0.233\phi_4 + 0.275\phi_5 - 0.308\phi_6 + 0.331\phi_7 - 0.342\phi_8 + 0.341\phi_9 - 0.328\phi_{10} + 0.304\phi_{11} - 0.270\phi_{12} + 0.26\phi_{13} - 0.174\phi_{14} + 0.117\phi_{15} - 0.055\phi_{16}$$

### a.3. Indeks kereaktifan

#### a.3.1. Pada Keadaan dasar

##### - Kerapatan Elektron

Kerapatan Elektron ( $q$ ) dihitung dengan menggunakan persamaan  $q = \sum_r n_r (c_{jr})^2$

$$q_1 = 2 \cdot (0.063)^2 + 2 \cdot (0.124)^2 + 2 \cdot (0.181)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.330)^2 + 2 \cdot (0.342)^2 \text{ solve, } q_1 \rightarrow 1.001312$$

$$q_2 = 2 \cdot (0.124)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.342)^2 + 2 \cdot (0.330)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.181)^2 + 2 \cdot (0.064)^2 \text{ solve, } q_2 \rightarrow 1.001566$$

$$q_3 = 2 \cdot (0.182)^2 + 2 \cdot (0.308)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.123)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (-0.231)^2 + 2 \cdot (-0.330)^2 \text{ solve, } q_3 \rightarrow 1.000568$$

$$q_4 = 2 \cdot (0.231)^2 + 2 \cdot (0.342)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.064)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (0.307)^2 + 2 \cdot (-0.125)^2 \text{ solve, } q_4 \rightarrow 1.001342$$

$$q_5 = 2 \cdot (0.274)^2 + 2 \cdot (0.330)^2 + 2 \cdot (0.124)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.341)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.064)^2 + 2 \cdot (0.306)^2 \text{ solve, } q_5 \rightarrow .999178$$

$$q_6 = 2 \cdot (0.307)^2 + 2 \cdot (0.274)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.123)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.182)^2 \text{ solve, } q_6 \rightarrow 1.001358$$

$$q_7 = 2 \cdot (0.330)^2 + 2 \cdot (0.181)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.062)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.125)^2 + 2 \cdot (0.273)^2 \text{ solve, } q_7 \rightarrow .9991$$

$$q_8 = 2 \cdot (0.342)^2 + 2 \cdot (0.064)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (-0.125)^2 + 2 \cdot (0.308)^2 + 2 \cdot (0.182)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.228)^2 \text{ solve, } q_8 \rightarrow 1.000172$$

$$q_9 = 2 \cdot (0.342)^2 + 2 \cdot (0.0623)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (0.123)^2 + 2 \cdot (0.308)^2 + 2 \cdot (-0.179)^2 + 2 \cdot (0.275)^2 + 2 \cdot (0.229)^2 \text{ solve, } q_9 \rightarrow .99969058$$

$$q_{10} = 2 \cdot (0.330)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.306)^2 + 2 \cdot (0.065)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.125)^2 + 2 \cdot (-0.275)^2 \text{ solve, } q_{10} \rightarrow 1.002398$$

$$q_{11} = 2 \cdot (0.274)^2 + 2 \cdot (-0.273)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (0.330)^2 + 2 \cdot (-0.238)^2 + 2 \cdot (-0.186)^2 + 2 \cdot (0.342)^2 + 2 \cdot (-0.178)^2 \text{ solve, } q_{11} \rightarrow 1.004978$$

$$q_{12} = 2 \cdot (0.231)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (0.193)^2 + 2 \cdot (0.182)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.229)^2 + 2 \cdot (0.066)^2 + 2 \cdot (0.308)^2 \text{ solve, } q_{12} \rightarrow 1.002518$$

$$q_{13} = 2 \cdot (-0.342)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.273)^2 + 2 \cdot (-0.062)^2 + 2 \cdot (-0.182)^2 + 2 \cdot (0.331)^2 + 2 \cdot (-0.306)^2 + 2 \cdot (0.121)^2 \text{ solve, } q_{13} \rightarrow .99932$$

$$q_{14} = 2 \cdot (0.182)^2 + 2 \cdot (-0.307)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.122)^2 + 2 \cdot (0.066)^2 + 2 \cdot (-0.233)^2 + 2 \cdot (0.331)^2 \text{ solve, } q_{14} \rightarrow 1.002546$$

$$q_{15} = 2 \cdot (0.124)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.308)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.329)^2 + 2 \cdot (-0.273)^2 + 2 \cdot (0.18)^2 + 2 \cdot (0.06)^2 \text{ solve, } q_{15} \rightarrow .999596$$

$$q_{16} = 2 \cdot (0.063)^2 + 2 \cdot (-0.125)^2 + 2 \cdot (0.182)^2 + 2 \cdot (-0.233)^2 + 2 \cdot (0.275)^2 + 2 \cdot (-0.308)^2 + 2 \cdot (0.331)^2 + 2 \cdot (0.342)^2 \text{ solve, } q_{16} \rightarrow 1.008042$$

- Orde ikatan (P)

Orde ikatan dilihat dengan menggunakan persamaan :  $P_{12} = \sum_j a_j c_j x_j^2$

$$\begin{aligned}
 P_{12} &= 2(0.0630.124) + 2(0.124.0.231) + 2(0.182.0.308) + 2(0.231.0.342) + 2(0.274.0.330) + 2(0.307.0.274) + 2(0.330.0.181) + 2(0.342.0.064) \rightarrow P_{12} = .85534 \\
 P_{23} &= 2(0.1810.124) + 2(0.307.0.231) + 2(0.341.0.308) + 2(0.274.0.342) + 2(0.124.0.330) + 2(-0.064.0.274) + 2(0.231.0.181) + 2(-0.330.0.064) \rightarrow P_{23} = .672344 \\
 P_{27} &= 2(0.330.0.124) + 2(0.181.0.231) + 2(-0.231.0.308) + 2(0.307.0.342) + 2(-0.062.0.330) + 2(-0.341.0.274) + 2(0.125.0.181) + 2(0.273.0.064) \rightarrow P_{27} = .541136 \\
 P_{34} &= 2(0.1810.231) + 2(-0.307.0.342) + 2(0.181.0.273) + 2(-0.341.0.273) + 2(0.274.0.056) + 2(0.124.0.180) + 2(-0.064.0.330) + 2(0.231.0.307) + 2(-0.330.0.125) \rightarrow P_{34} = .736802 \\
 P_{45} &= 2(0.274.0.231) + 2(0.330.0.342) + 2(0.123.0.273) + 2(-0.232.0.273) + 2(-0.180.0.064) + 2(-0.341.0.180) + 2(-0.062.0.307) + 2(0.308.0.125) \rightarrow P_{45} = .633374 \\
 P_{56} &= 2(0.274.0.307) + 2(-0.330.0.274) + 2(0.123.-0.064) + 2(-0.130.-0.330) + 2(-0.341.-0.232) + 2(-0.232.0.123) + 2(0.062.0.341) + 2(-0.308.0.182) \rightarrow P_{56} = .70763 \\
 P_{67} &= 2(0.330.0.307) + 2(0.181.0.274) + 2(-0.231.-0.064) + 2(-0.307.-0.330) + 2(0.062.-0.232) + 2(0.341.0.123) + 2(0.125.0.341) + 2(-0.223.0.182) \rightarrow P_{67} = .574992 \\
 P_{58} &= 2(0.274.0.342) + 2(0.330.0.064) + 2(0.123.-0.330) + 2(-0.180.-0.123) + 2(-0.341.0.306) + 2(-0.062.0.273) + 2(0.062.0.273) + 2(-0.308.0.223) \rightarrow P_{58} = .071556 \\
 P_{89} &= 2(0.342.0.342) + 2(0.062.0.064) + 2(-0.330.-0.330) + 2(0.123.-0.123) + 2(0.308.0.306) + 2(-0.179.0.182) + 2(-0.275.0.273) + 2(-0.229.0.223) \rightarrow P_{89} = .504238 \\
 P_{910} &= 2(0.342.0.330) + 2(0.062.-0.181) + 2(-0.330.-0.232) + 2(0.123.0.506) + 2(0.308.0.061) + 2(-0.179.-0.342) + 2(-0.225.0.122) + 2(0.229.0.275) \rightarrow P_{910} = .652993 \\
 P_{914} &= 2(0.342.0.181) + 2(0.062.0.307) + 2(-0.330.-0.341) + 2(0.123.0.273) + 2(0.308.0.122) + 2(-0.179.0.066) + 2(-0.275.-0.232) + 2(0.229.0.331) \rightarrow P_{914} = .7855562 \\
 P_{1011} &= 2(0.307.0.330) + 2(-0.275.-0.181) + 2(-0.064.-0.232) + 2(-0.330.0.306) + 2(-0.230.0.065) + 2(-0.125.-0.342) + 2(0.342.0.122) + 2(-0.178.0.275) \rightarrow P_{1011} = .574934 \\
 P_{1112} &= 2(0.307.0.274) + 2(-0.273.-0.330) + 2(-0.064.0.123) + 2(0.330.0.182) + 2(-0.126.0.229) + 2(-0.342..0.066) + 2(-0.173.-0.368) \rightarrow P_{1112} = .616908 \\
 P_{1213} &= 2(0.221.0.274) + 2(-0.342.-0.330) + 2(0.273.0.123) + 2(-0.061.0.182) + 2(-0.132..0.342) + 2(0.331.0.229) + 2(0.305..0.066) + 2(0.121..0.308) \rightarrow P_{1213} = .55342 \\
 P_{1314} &= 2(0.231.0.181) + 2(-0.342..0.307) + 2(0.273.0.341) + 2(-0.051.-0.273) + 2(-0.182.0.122) + 2(0.331.-0.056) + 2(0.306.0.233) + 2(0.121.0.331) \rightarrow P_{1314} = .6477 \\
 P_{1415} &= 2(-0.124.0.181) + 2(-0.232.-0.307) + 2(0.308.0.341) + 2(-0.342..0.273) + 2(0.329.0.122) + 2(-0.272.-0.055) + 2(0.178.0.233) \rightarrow P_{1415} = .624418 \\
 P_{1516} &= 2(-0.124.0.663) + 2(-0.232.-0.125) + 2(0.308.0.182) + 2(-0.342..0.233) + 2(0.329.0.275) + 2(-0.272.-0.308) + 2(0.178.0.331) + 2(-0.059.-0.242) \rightarrow P_{1516} = .820554
 \end{aligned}$$

- Harga valensi

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.855 \text{ solve}, F_1 \rightarrow .8770508075688772935$$

$$F_2 = \sqrt{3} - 0.855 - 0.672 - 0.541 \text{ solve}, F_2 \rightarrow -.3359491924311227065$$

$$F_3 = \sqrt{3} - 0.672 - 0.737 \text{ solve}, F_3 \rightarrow .3230508075688772935$$

$$F_4 = \sqrt{3} - 0.737 - 0.633 \text{ solve}, F_4 \rightarrow .3620508075688772935$$

$$F_5 = \sqrt{3} - 0.633 - 0.708 - 0.0715 \text{ solve}, F_5 \rightarrow .3195508075688772935$$

$$F_6 = \sqrt{3} - 0.708 - 0.575 \text{ solve}, F_6 \rightarrow .4490508075688772935$$

$$F_7 = \sqrt{3} - 0.541 - 0.575 \text{ solve}, F_7 \rightarrow .6160508075688772935$$

$$F_8 = \sqrt{3} - 0.0715 - 0.504 \text{ solve}, F_8 \rightarrow 1.1565508075688772935$$

$$F_9 = \sqrt{3} - 0.504 - 0.653 - 0.785 \text{ solve}, F_9 \rightarrow -.2099491924311227065$$

$$F_{10} = \sqrt{3} - 0.653 - 0.575 \text{ solve}, F_{10} \rightarrow .5040508075688772935$$

$$F_{11} = \sqrt{3} - 0.575 - 0.517 \text{ solve}, F_{11} \rightarrow .6400508075688772935$$

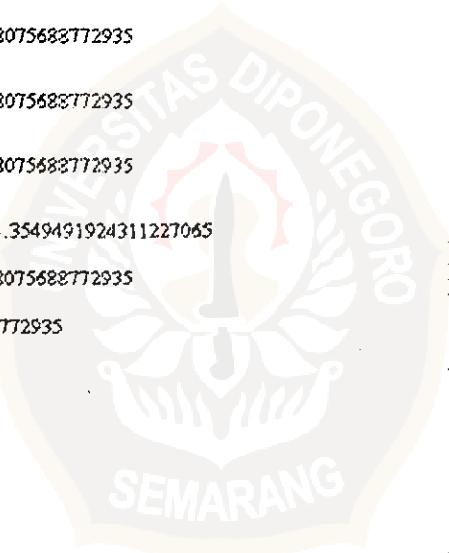
$$F_{12} = \sqrt{3} - 0.517 - 0.558 \text{ solve}, F_{12} \rightarrow .6570508075688772935$$

$$F_{13} = \sqrt{3} - 0.558 - 0.648 \text{ solve}, F_{13} \rightarrow .5260508075688772935$$

$$F_{14} = \sqrt{3} - 0.648 - 0.785 - 0.654 \text{ solve}, F_{14} \rightarrow -.3549491924311227065$$

$$F_{15} = \sqrt{3} - 0.654 - 0.820 \text{ solve}, F_{15} \rightarrow .2580508075688772935$$

$$F_{16} = \sqrt{3} - 0.820 \text{ solve}, F_{16} \rightarrow .9120508075688772935$$



### 3.3.2. Pada Keadaan tereksitasi

A. Elektron Tereksitasi ke 1 Tingkat Energi lebih tinggi

#### - Kerapatan Elektron (q)

$$\begin{aligned} q_1 &= 2 \cdot (0.063)^2 + 2 \cdot (0.124)^2 - 2 \cdot (0.181)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.330)^2 + (0.342)^2 + (0.342)^2 \text{ solve, } q_1 \rightarrow 1.001312 \\ q_2 &= 2 \cdot (0.124)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.342)^2 + 2 \cdot (0.330)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.181)^2 + (0.064)^2 + (0.062)^2 \text{ solve, } q_2 \rightarrow 1.001314 \\ q_3 &= 2 \cdot (0.182)^2 + 2 \cdot (0.308)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.123)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (-0.221)^2 + (-0.330)^2 + (-0.330)^2 \text{ solve, } q_3 \rightarrow 1.000568 \\ q_4 &= 2 \cdot (0.231)^2 + 2 \cdot (0.342)^2 + 2 \cdot (0.274)^2 + 2 \cdot (0.064)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.125)^2 + (0.123)^2 \text{ solve, } q_4 \rightarrow 1.000846 \\ q_5 &= 2 \cdot (0.274)^2 + 2 \cdot (0.350)^2 + 2 \cdot (0.124)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.341)^2 + 2 \cdot (0.064)^2 + (0.306)^2 + (0.308)^2 \text{ solve, } q_5 \rightarrow 1.000406 \\ q_6 &= 2 \cdot (0.307)^2 + 2 \cdot (0.274)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.123)^2 + 2 \cdot (0.341)^2 + (0.152)^2 + (-0.179)^2 \text{ solve, } q_6 \rightarrow 1.000275 \\ q_7 &= 2 \cdot (0.330)^2 + 2 \cdot (0.181)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.307)^2 + 2 \cdot (0.062)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.125)^2 + (0.275)^2 + (0.275)^2 \text{ solve, } q_7 \rightarrow 1.000196 \\ q_8 &= 2 \cdot (0.342)^2 + 2 \cdot (0.064)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (-0.125)^2 + 2 \cdot (0.308)^2 + 2 \cdot (-0.132)^2 + 2 \cdot (0.273)^2 + (0.222)^2 + (0.222)^2 \text{ solve, } q_8 \rightarrow 1.0006529 \\ q_9 &= 2 \cdot (0.342)^2 + 2 \cdot (0.0623)^2 + 2 \cdot (-0.530)^2 + 2 \cdot (0.123)^2 + 2 \cdot (0.308)^2 + 2 \cdot (-0.179)^2 + 2 \cdot (0.275)^2 + (0.225)^2 + (0.235)^2 \text{ solve, } q_9 \rightarrow 1.00153858 \\ q_{10} &= 2 \cdot (0.330)^2 + 2 \cdot (-0.180)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.306)^2 + 2 \cdot (0.065)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.125)^2 + (-0.275)^2 + (-0.275)^2 \text{ solve, } q_{10} \rightarrow 1.0009757 \\ q_{11} &= 2 \cdot (0.274)^2 + 2 \cdot (-0.273)^2 + 2 \cdot (-0.064)^2 + 2 \cdot (0.330)^2 + 2 \cdot (-0.238)^2 + 2 \cdot (-0.186)^2 + 2 \cdot (0.342)^2 + (-0.178)^2 + (-0.183)^2 \text{ solve, } q_{11} \rightarrow 1.006783 \\ q_{12} &= 2 \cdot (0.231)^2 + 2 \cdot (-0.330)^2 + 2 \cdot (0.193)^2 + 2 \cdot (0.152)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.229)^2 + 2 \cdot (0.055)^2 + (0.308)^2 + (0.305)^2 \text{ solve, } q_{12} \rightarrow 1.0006579 \\ q_{13} &= 2 \cdot (0.342)^2 + 2 \cdot (0.231)^2 + 2 \cdot (0.273)^2 + 2 \cdot (-0.062)^2 + 2 \cdot (-0.062)^2 + 2 \cdot (-0.182)^2 + 2 \cdot (0.331)^2 + 2 \cdot (-0.305)^2 + (0.121)^2 + (0.127)^2 \text{ solve, } q_{13} \rightarrow 1.0000808 \\ q_{14} &= 2 \cdot (0.182)^2 + 2 \cdot (-0.307)^2 + 2 \cdot (0.341)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.122)^2 + 2 \cdot (0.056)^2 + 2 \cdot (-0.233)^2 + (0.331)^2 + (-0.239)^2 \text{ solve, } q_{14} \rightarrow 1.001226 \\ q_{15} &= 2 \cdot (0.124)^2 + 2 \cdot (-0.232)^2 + 2 \cdot (0.308)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (0.329)^2 + 2 \cdot (-0.342)^2 + 2 \cdot (-0.273)^2 + 2 \cdot (0.18)^2 + (0.06)^2 + (0.06)^2 \text{ solve, } q_{15} \rightarrow 1.0004985 \\ q_{16} &= 2 \cdot (0.063)^2 + 2 \cdot (-0.125)^2 + 2 \cdot (0.125)^2 + 2 \cdot (-0.233)^2 + 2 \cdot (0.182)^2 + 2 \cdot (0.275)^2 + 2 \cdot (-0.233)^2 + 2 \cdot (0.331)^2 + 2 \cdot (-0.308)^2 + (0.342)^2 + (0.341)^2 \text{ solve, } q_{16} \rightarrow 1.007359 \end{aligned}$$

### - Orde ikatan

$$P_{12}=2(0.063-0.124)+2\cdot(0.124-0.231)+2\cdot(0.182-0.308)+2\cdot(0.231-0.342)+2\cdot(0.274-0.330)+2\cdot(0.307-0.274)+2\cdot(0.330-0.181)+1\cdot(0.342-0.064)+1\cdot(0.342-0.062)\rightarrow P_{12}=.8546556$$

$$P_{23}=2(0.181-0.124)+2\cdot(0.307-0.231)+2\cdot(0.341-0.308)+2\cdot(0.274-0.342)+2\cdot(0.124-0.330)+2\cdot(-0.064-0.274)+2\cdot(0.221-0.181)+1\cdot(-0.330-0.064)+1\cdot(-0.330-0.062)\rightarrow P_{23}=.673094$$

$$P_{24}=2(-0.330-0.124)+2\cdot(0.181-0.231)+2\cdot(-0.231-0.308)+2\cdot(0.062-0.330)+2\cdot(0.307-0.242)+2\cdot(0.125-0.274)+2\cdot(0.125-0.181)+1\cdot(0.273-0.064)+1\cdot(0.275-0.062)\rightarrow P_{27}=.546714$$

$$P_{45}=2(0.181-0.231)+2\cdot(0.307-0.342)+2\cdot(0.341-0.273)+2\cdot(0.274-0.064)+2\cdot(0.274-0.330)+2\cdot(-0.064-0.330)+2\cdot(0.124-0.180)+2\cdot(0.125-0.125)+1\cdot(-0.330-0.123)\rightarrow P_{34}=.654962$$

$$P_{56}=2(0.274-0.231)+2\cdot(0.350-0.342)+2\cdot(0.123-0.273)+2\cdot(-0.180-0.064)+2\cdot(-0.341-0.180)+2\cdot(0.062-0.307)+2\cdot(0.232-0.330)+1\cdot(0.308-0.125)+1\cdot(0.308-0.123)\rightarrow P_{45}=.709758$$

$$P_{56}=2(-0.274-0.307)+2\cdot(-0.330-0.274)+2\cdot(0.123-0.064)+2\cdot(-0.180-0.330)+2\cdot(-0.341-0.232)+2\cdot(-0.232-0.123)+2\cdot(0.062-0.341)+1\cdot(0.308-0.182)+1\cdot(0.308-0.179)\rightarrow P_{56}=.593492$$

$$P_{67}=2(-0.330-0.307)+2\cdot(0.181-0.274)+2\cdot(-0.231-0.064)+2\cdot(-0.307-0.330)+2\cdot(-0.662-0.232)+2\cdot(0.124-0.123)+2\cdot(-0.273-0.182)+1\cdot(-0.275-0.179)\rightarrow P_{67}=.673903$$

$$P_{58}=2(0.274-0.342)+2\cdot(0.350-0.064)+2\cdot(0.123-0.330)+2\cdot(-0.120-0.125)+2\cdot(-0.341-0.306)+2\cdot(-0.232-0.182)+2\cdot(0.062-0.273)+1\cdot(0.308-0.223)+1\cdot(0.308-0.229)\rightarrow P_{58}=.073464$$

$$P_{89}=2(0.342-0.342)+2\cdot(0.062-0.064)+2\cdot(-0.330-0.330)+2\cdot(0.123-0.125)+2\cdot(0.308-0.306)+2\cdot(-0.179-0.182)+2\cdot(-0.275-0.273)+1\cdot(0.233-0.229)\rightarrow P_{89}=.506528$$

$$P_{910}=2(0.342-0.330)+2\cdot(0.062-0.181)+2\cdot(-0.330-0.232)+2\cdot(0.123-0.273)+2\cdot(-0.179-0.342)+2\cdot(-0.275-0.122)+1\cdot(0.229-0.273)+1\cdot(0.233-0.272)\rightarrow P_{910}=.653399$$

$$P_{914}=2(0.342-0.181)+2\cdot(0.062-0.307)+2\cdot(-0.330-0.341)+2\cdot(0.123-0.273)+2\cdot(-0.179-0.265)+2\cdot(-0.275-0.233)+1\cdot(0.229-0.331)+1\cdot(0.233-0.238)\rightarrow P_{914}=.6533876$$

$$P_{1011}=2(0.307-0.330)+2\cdot(-0.273-0.181)+2\cdot(-0.064-0.232)+2\cdot(0.330-0.306)+2\cdot(-0.230-0.065)+2\cdot(-0.125-0.342)+2\cdot(0.342-0.122)+1\cdot(-0.178-0.275)+1\cdot(-0.183-0.272)\rightarrow P_{1011}=.67366$$

$$P_{1112}=2(0.307-0.274)+2\cdot(-0.273-0.330)+2\cdot(-0.064-0.122)+2\cdot(0.350-0.182)+2\cdot(-0.230-0.342)+2\cdot(-0.125-0.229)+2\cdot(-0.342-0.066)+1\cdot(-0.178-0.308)+1\cdot(0.183-0.305)\rightarrow P_{1112}=.617899$$

$$P_{1213}=2(0.231-0.274)+2\cdot(-0.342-0.330)+2\cdot(-0.273-0.123)+2\cdot(-0.061-0.182)+2\cdot(-0.182-0.242)+2\cdot(0.331-0.229)+2\cdot(-0.306-0.066)+1\cdot(0.121-0.305)+1\cdot(0.127-0.305)\rightarrow P_{1213}=.634423$$

$$P_{1314}=2(0.231-0.181)+2\cdot(-0.342-0.307)+2\cdot(-0.273-0.341)+2\cdot(-0.061-0.273)+2\cdot(-0.182-0.122)+2\cdot(0.331-0.066)+2\cdot(0.306-0.233)+1\cdot(0.121-0.331)+1\cdot(0.127-0.239)\rightarrow P_{1314}=.638002$$

$$P_{1415}=2(-0.124-0.181)+2\cdot(-0.232-0.307)+2\cdot(0.308-0.341)+2\cdot(-0.342-0.273)+2\cdot(-0.329-0.122)+2\cdot(-0.272-0.066)+2\cdot(0.178-0.233)+1\cdot(-0.059-0.331)+1\cdot(-0.067-0.239)\rightarrow P_{1415}=.657934$$

$$P_{1516}=2(-0.124-0.063)+2\cdot(-0.252-0.125)+2\cdot(0.308-0.182)+2\cdot(-0.342-0.233)+2\cdot(-0.329-0.275)+2\cdot(0.178-0.331)+1\cdot(-0.059-0.342)+1\cdot(-0.087-0.341)\rightarrow P_{1516}=.777529$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.859 \text{ solve}, F_1 \rightarrow .8730508075688772935$$

$$F_2 = \sqrt{3} - 0.859 - 0.673 - 0.541 \text{ solve}, F_2 \rightarrow -.3409491924311227065$$

$$F_3 = \sqrt{3} - 0.673 - 0.655 \text{ solve}, F_3 \rightarrow .4040508075688772935$$

$$F_4 = \sqrt{3} - 0.655 - 0.709 \text{ solve}, F_4 \rightarrow .3680508075688772935$$

$$F_5 = \sqrt{3} - 0.709 - 0.596 - 0.073 \text{ solve}, F_5 \rightarrow .3540508075688772935$$

$$F_6 = \sqrt{3} - 0.596 - 0.674 \text{ solve}, F_6 \rightarrow .4620508075688772935$$

$$F_7 = \sqrt{3} - 0.541 - 0.674 \text{ solve}, F_7 \rightarrow .5170508075688772935$$

$$F_8 = \sqrt{3} - 0.073 - 0.596 \text{ solve}, F_8 \rightarrow 1.0630508075688772935$$

$$F_9 = \sqrt{3} - 0.596 - 0.653 - 0.654 \text{ solve}, F_9 \rightarrow -.1709491924311227065$$

$$F_{10} = \sqrt{3} - 0.653 - 0.673 \text{ solve}, F_{10} \rightarrow .4060508075688772935$$

$$F_{11} = \sqrt{3} - 0.673 - 0.618 \text{ solve}, F_{11} \rightarrow .4410508075688772935$$

$$F_{12} = \sqrt{3} - 0.618 - 0.639 \text{ solve}, F_{12} \rightarrow .4750508075688772935$$

$$F_{13} = \sqrt{3} - 0.639 - 0.638 \text{ solve}, F_{13} \rightarrow .4550508075688772935$$

$$F_{14} = \sqrt{3} - 0.638 - 0.657 - 0.654 \text{ solve}, F_{14} \rightarrow -.2169491924311227065$$

$$F_{15} = \sqrt{3} - 0.657 - 0.778 \text{ solve}, F_{15} \rightarrow .2970508075688772935$$

$$F_{16} = \sqrt{3} - 0.778 \text{ solve}, F_{16} \rightarrow .9540508075688772935$$

## B. 1 Elektron tereksitasi ke 2 tingkat energi lebih tinggi -Kerapatan elektron { q }

$$\begin{aligned}
 q_1 &= 2(0.063)^2 + 2(0.124)^2 + 2(-0.181)^2 + 2(0.231)^2 + 2(0.274)^2 + 2(0.307)^2 + 2(0.330)^2 + 2(0.350)^2 + 2(0.367)^2 + (0.342)^2 + (0.330)^2 \text{ solve, } q_1 \rightarrow .933248 \\
 q_2 &= 2(0.124)^2 + 2(0.231)^2 + 2(0.307)^2 + 2(0.342)^2 + 2(0.330)^2 + 2(0.274)^2 + 2(-0.181)^2 + 2(0.131)^2 + (0.054)^2 + (-0.182)^2 \text{ solve, } q_2 \rightarrow 1.02987 \\
 q_3 &= 2(0.182)^2 + 2(0.308)^2 + 2(-0.341)^2 + 2(0.273)^2 + 2(0.123)^2 + 2(-0.054)^2 + 2(-0.231)^2 + 2(-0.23)^2 + (-0.330)^2 + (-0.232)^2 \text{ solve, } q_3 \rightarrow .945492 \\
 q_4 &= 2(0.231)^2 + 2(0.342)^2 + 2(0.274)^2 + 2(-0.054)^2 + 2(-0.180)^2 + 2(-0.330)^2 + 2(0.307)^2 + 2(0.339)^2 + 2(-0.23)^2 + (0.306)^2 + (0.305)^2 \text{ solve, } q_4 \rightarrow 1.079353 \\
 q_5 &= 2(0.274)^2 + 2(0.330)^2 + 2(-0.180)^2 + 2(-0.124)^2 + 2(-0.180)^2 + 2(-0.341)^2 + 2(-0.232)^2 + 2(0.054)^2 + (0.395)^2 + (0.065)^2 \text{ solve, } q_5 \rightarrow .909767 \\
 q_6 &= 2(0.307)^2 + 2(0.274)^2 + 2(-0.054)^2 + 2(-0.330)^2 + 2(-0.232)^2 + 2(0.123)^2 + 2(0.341)^2 + (0.182)^2 + (-0.182)^2 + (0.342)^2 \text{ solve, } q_6 \rightarrow 1.085193 \\
 q_7 &= 2(0.330)^2 + 2(-0.181)^2 + 2(0.231)^2 + 2(0.307)^2 + 2(0.062)^2 + 2(-0.341)^2 + 2(0.125)^2 + (0.273)^2 + (0.122)^2 \text{ solve, } q_7 \rightarrow .939455 \\
 q_8 &= 2(0.342)^2 + 2(-0.064)^2 + 2(-0.530)^2 + 2(-0.125)^2 + 2(-0.308)^2 + 2(0.123)^2 + 2(-0.175)^2 + 2(0.273)^2 + (0.228)^2 + (-0.234)^2 \text{ solve, } q_8 \rightarrow 1.023313 \\
 q_9 &= 2(0.342)^2 + 2(0.0623)^2 + 2(-0.330)^2 + 2(0.123)^2 + 2(0.308)^2 + 2(-0.175)^2 + 2(0.273)^2 + (0.228)^2 + (-0.234)^2 \text{ solve, } q_9 \rightarrow 1.02123358 \\
 q_{10} &= 2(0.330)^2 + 2(-0.180)^2 + 2(-0.232)^2 + 2(0.306)^2 + 2(0.065)^2 + 2(-0.342)^2 + 2(0.125)^2 + (-0.225)^2 + (-0.225)^2 \text{ solve, } q_{10} \rightarrow .999673 \\
 q_{11} &= 2(0.234)^2 + 2(-0.273)^2 + 2(-0.054)^2 + 2(0.330)^2 + 2(-0.238)^2 + 2(-0.186)^2 + 2(0.342)^2 + (-0.178)^2 + (0.341)^2 \text{ solve, } q_{11} \rightarrow 1.089575 \\
 q_{12} &= 2(0.231)^2 + 2(-0.350)^2 + 2(0.193)^2 + 2(0.182)^2 + 2(-0.342)^2 + 2(0.229)^2 + 2(0.056)^2 + (0.368)^2 + (-0.059)^2 \text{ solve, } q_{12} \rightarrow .911135 \\
 q_{13} &= 2(-0.342)^2 + 2(0.231)^2 + 2(-0.273)^2 + 2(-0.062)^2 + 2(-0.182)^2 + 2(0.331)^2 + 2(-0.306)^2 + (0.121)^2 + (-0.309)^2 \text{ solve, } q_{13} \rightarrow 1.08016 \\
 q_{14} &= 2(0.182)^2 + 2(-0.307)^2 + 2(-0.341)^2 + 2(0.273)^2 + 2(-0.122)^2 + 2(0.056)^2 + 2(-0.233)^2 + (0.331)^2 + (0.228)^2 \text{ solve, } q_{14} \rightarrow .944969 \\
 q_{15} &= 2(0.124)^2 + 2(-0.232)^2 + 2(-0.308)^2 + 2(-0.342)^2 + 2(0.329)^2 + 2(-0.273)^2 + 2(0.18)^2 + (0.06)^2 + (0.185)^2 \text{ solve, } q_{15} \rightarrow 1.030221 \\
 q_{16} &= 2(0.063)^2 + 2(-0.125)^2 + 2(0.182)^2 + 2(-0.233)^2 + 2(0.275)^2 + 2(-0.308)^2 + 2(0.331)^2 + (0.331)^2 + (-0.238)^2 + (-0.242)^2 \text{ solve, } q_{16} \rightarrow .947722
 \end{aligned}$$

### - Orde ikatan

$$P_{12}=2\cdot(0.003\cdot0.124)+2\cdot(0.122\cdot0.231)+2\cdot(0.122\cdot0.308)+2\cdot(0.231\cdot0.342)+2\cdot(0.274\cdot0.330)+2\cdot(0.307\cdot0.274)+2\cdot(0.330\cdot0.181)+1\cdot(0.242\cdot0.064)+1\cdot(0.330\cdot0.180)\rightarrow P_{12}=.774052$$

$$P_{23}=2\cdot(0.181\cdot0.124)+2\cdot(0.307\cdot0.231)+2\cdot(0.341\cdot0.308)+2\cdot(0.274\cdot0.342)+2\cdot(0.124\cdot0.330)+2\cdot(0.124\cdot0.274)+2\cdot(0.231\cdot0.181)+1\cdot(-0.330\cdot0.064)+1\cdot(-0.180\cdot0.232)\rightarrow P_{23}=.735224$$

$$P_{27}=2\cdot(0.330\cdot0.124)+2\cdot(0.131\cdot0.231)+2\cdot(-0.221\cdot0.308)+2\cdot(0.307\cdot0.342)+2\cdot(0.052\cdot0.330)+2\cdot(0.341\cdot0.274)+2\cdot(0.125\cdot0.181)+1\cdot(0.273\cdot0.064)+1\cdot(-0.180\cdot0.122)\rightarrow P_{27}=.501704$$

$$P_{34}=2\cdot(0.181\cdot0.231)+2\cdot(0.307\cdot0.342)+2\cdot(0.341\cdot0.273)+2\cdot(0.274\cdot0.064)+2\cdot(0.124\cdot0.180)+2\cdot(-0.064\cdot0.330)+2\cdot(0.231\cdot0.307)+1\cdot(-0.330\cdot0.125)+1\cdot(-0.222\cdot0.306)\rightarrow P_{34}=.62456$$

$$P_{45}=2\cdot(0.274\cdot0.231)+2\cdot(0.330\cdot0.342)+2\cdot(0.123\cdot0.273)+2\cdot(0.274\cdot0.330)+2\cdot(-0.341\cdot0.180)+2\cdot(-0.341\cdot0.064)+2\cdot(0.062\cdot0.307)+1\cdot(0.308\cdot0.125)+1\cdot(0.306\cdot0.065)\rightarrow P_{45}=.691764$$

$$P_{56}=2\cdot(0.274\cdot0.307)+2\cdot(0.350\cdot0.274)+2\cdot(0.123\cdot0.064)+2\cdot(-0.120\cdot0.330)+2\cdot(-0.064\cdot0.232)+2\cdot(0.052\cdot0.341)+1\cdot(0.308\cdot0.132)+1\cdot(0.065\cdot0.342)\rightarrow P_{56}=.529334$$

$$P_{67}=2\cdot(0.330\cdot0.307)+2\cdot(0.131\cdot0.274)+2\cdot(-0.231\cdot0.064)+2\cdot(0.062\cdot0.232)+2\cdot(0.341\cdot0.123)+2\cdot(0.125\cdot0.341)+1\cdot(-0.273\cdot0.122)+1\cdot(-0.342\cdot0.122)\rightarrow P_{67}=.582294$$

$$P_{73}=2\cdot(0.274\cdot0.342)+2\cdot(0.330\cdot0.624)+2\cdot(0.123\cdot0.330)+2\cdot(-0.180\cdot0.125)+2\cdot(-0.341\cdot0.306)+2\cdot(0.052\cdot0.273)+2\cdot(0.232\cdot0.122)\rightarrow P_{73}=.015603$$

$$P_{78}=2\cdot(0.342\cdot0.342)+2\cdot(0.062\cdot0.664)+2\cdot(-0.330\cdot0.330)+2\cdot(0.123\cdot0.125)+2\cdot(0.308\cdot0.306)+2\cdot(-0.175\cdot0.182)+2\cdot(-0.275\cdot0.273)+1\cdot(0.229\cdot0.223)+1\cdot(-0.275\cdot0.272)\rightarrow P_{78}=.527971$$

$$P_{910}=2\cdot(0.342\cdot0.330)+2\cdot(0.062\cdot0.181)+2\cdot(-0.330\cdot0.232)+2\cdot(0.123\cdot0.306)+2\cdot(0.308\cdot0.065)+2\cdot(-0.179\cdot0.342)+2\cdot(-0.275\cdot0.122)+1\cdot(-0.270\cdot0.272)\rightarrow P_{910}=.663463$$

$$P_{914}=2\cdot(0.342\cdot0.181)+2\cdot(0.052\cdot0.307)+2\cdot(-0.330\cdot0.341)+2\cdot(0.123\cdot0.273)+2\cdot(0.308\cdot0.122)+2\cdot(-0.179\cdot0.365)+2\cdot(-0.275\cdot0.233)+1\cdot(0.229\cdot0.331)+1\cdot(-0.272\cdot0.228)\rightarrow P_{914}=.647547$$

$$P_{1011}=2\cdot(0.307\cdot0.330)+2\cdot(-0.275\cdot0.181)+2\cdot(-0.064\cdot0.232)+2\cdot(0.330\cdot0.305)+2\cdot(-0.230\cdot0.065)+2\cdot(-0.126\cdot0.342)+2\cdot(0.342\cdot0.122)+1\cdot(-0.178\cdot0.275)+1\cdot(0.341\cdot0.27)\rightarrow P_{1011}=.531814$$

$$P_{1112}=2\cdot(0.307\cdot0.274)+2\cdot(-0.275\cdot0.330)+2\cdot(-0.054\cdot0.123)+2\cdot(0.330\cdot0.182)+2\cdot(-0.230\cdot0.342)+2\cdot(-0.126\cdot0.225)+2\cdot(0.342\cdot0.066)+1\cdot(-0.178\cdot0.308)+1\cdot(0.341\cdot0.059)\rightarrow P_{1112}=.541965$$

$$P_{1213}=2\cdot(0.231\cdot0.274)+2\cdot(-0.343\cdot0.330)+2\cdot(0.273\cdot0.123)+2\cdot(-0.061\cdot0.182)+2\cdot(0.182\cdot0.342)+2\cdot(0.331\cdot0.229)+2\cdot(0.306\cdot0.066)+1\cdot(0.121\cdot0.308)+1\cdot(-0.059\cdot0.309)\rightarrow P_{1213}=.613319$$

$$P_{1314}=2\cdot(0.231\cdot0.181)+2\cdot(-0.342\cdot0.307)+2\cdot(0.273\cdot0.341)+2\cdot(-0.061\cdot0.273)+2\cdot(0.182\cdot0.122)+2\cdot(0.331\cdot0.066)+2\cdot(0.306\cdot0.233)+1\cdot(0.121\cdot0.331)+1\cdot(-0.309\cdot0.228)\rightarrow P_{1314}=.557197$$

$$P_{1415}=2\cdot(0.124\cdot0.181)+2\cdot(-0.252\cdot0.307)+2\cdot(0.308\cdot0.341)+2\cdot(-0.342\cdot0.273)+2\cdot(0.329\cdot0.122)+2\cdot(-0.272\cdot0.065)+2\cdot(0.178\cdot0.233)+1\cdot(-0.059\cdot0.331)+1\cdot(0.228\cdot0.185)\rightarrow P_{1415}=.716127$$

$$P_{1516}=2\cdot(0.124\cdot0.063)+2\cdot(-0.222\cdot0.125)+2\cdot(0.308\cdot0.182)+2\cdot(-0.342\cdot0.233)+2\cdot(0.329\cdot0.275)+2\cdot(-0.272\cdot0.308)+2\cdot(0.178\cdot0.311)+1\cdot(-0.059\cdot0.342)+1\cdot(0.185\cdot0.238)\rightarrow P_{1516}=.756346$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.774 \text{ solve}, F_1 \rightarrow .9580508075688772935$$

$$F_2 = \sqrt{3} - 0.774 - 0.735 - 0.502 \text{ solve}, F_2 \rightarrow -.2789491924311227065$$

$$F_3 = \sqrt{3} - 0.735 - 0.625 \text{ solve}, F_3 \rightarrow .3720508075688772935$$

$$F_4 = \sqrt{3} - 0.625 - 0.692 \text{ solve}, F_4 \rightarrow .4150508075688772935$$

$$F_5 = \sqrt{3} - 0.692 - 0.629 - -0.015 \text{ solve}, F_5 \rightarrow .4260508075688772935$$

$$F_6 = \sqrt{3} - 0.629 - 0.583 \text{ solve}, F_6 \rightarrow .5200508075688772935$$

$$F_7 = \sqrt{3} - 0.502 - 0.583 \text{ solve}, F_7 \rightarrow .6470508075688772935$$

$$F_8 = \sqrt{3} - -0.015 - 0.528 \text{ solve}, F_8 \rightarrow 1.2190508075688772935$$

$$F_9 = \sqrt{3} - 0.528 - 0.663 - 0.647 \text{ solve}, F_9 \rightarrow -.1059491924311227065$$

$$F_{10} = \sqrt{3} - 0.663 - 0.532 \text{ solve}, F_{10} \rightarrow .5370508075688772935$$

$$F_{11} = \sqrt{3} - 0.532 - -0.512 \text{ solve}, F_{11} \rightarrow .6580508075688772935$$

$$F_{12} = \sqrt{3} - 0.542 - 0.614 \text{ solve}, F_{12} \rightarrow .5760508075688772935$$

$$F_{13} = \sqrt{3} - 0.614 - 0.537 \text{ solve}, F_{13} \rightarrow .5810508075688772935$$

$$F_{14} = \sqrt{3} - 0.647 - 0.716 - 0.537 \text{ solve}, F_{14} \rightarrow -.1679491924311227065$$

$$F_{15} = \sqrt{3} - 0.716 - 0.756 \text{ solve}, F_{15} \rightarrow .2600508075688772935$$

$$F_{16} = \sqrt{3} - 0.756 \text{ solve}, F_{16} \rightarrow .9760508075688772935$$



### C. 1 Elektron teriksasi ke 3 tingkat energi lebih tinggi .

#### - Kerapatan elektron ( q ) .

$$q_1=2\cdot(0.063)^2+2\cdot(0.124)^2+2\cdot(0.181)^2+2\cdot(0.231)^2+2\cdot(0.274)^2+2\cdot(0.307)^2+2\cdot(0.330)^2+2\cdot(0.364)^2+(0.342)^2+(0.374)^2 \text{ solve, } q_1 \rightarrow .959424$$

$$q_2=2\cdot(0.124)^2+2\cdot(0.231)^2+2\cdot(0.307)^2+2\cdot(0.342)^2+2\cdot(0.330)^2+2\cdot(0.274)^2+2\cdot(0.181)^2+2\cdot(0.274)^2+2\cdot(0.064)^2+(0.064)^2+(-0.273)^2 \text{ solve, } q_2 \rightarrow 1.071999$$

$$q_3=2\cdot(0.182)^2+2\cdot(0.308)^2+2\cdot(0.341)^2+2\cdot(0.273)^2+2\cdot(0.123)^2+2\cdot(-0.064)^2+2\cdot(-0.231)^2+(-0.330)^2+(-0.330)^2+(-0.064)^2 \text{ solve, } q_3 \rightarrow .885764$$

$$q_4=2\cdot(0.231)^2+2\cdot(0.124)^2+2\cdot(0.274)^2+2\cdot(0.064)^2+2\cdot(-0.180)^2+2\cdot(-0.330)^2+2\cdot(0.307)^2+2\cdot(0.125)^2+(0.330)^2 \text{ solve, } q_4 \rightarrow 1.094617$$

$$q_5=2\cdot(0.274)^2+2\cdot(0.330)^2+2\cdot(0.124)^2+2\cdot(0.180)^2+2\cdot(-0.341)^2+2\cdot(-0.232)^2+2\cdot(0.064)^2+(0.305)^2+(0.230)^2 \text{ solve, } q_5 \rightarrow .958442$$

$$q_6=2\cdot(0.307)^2+2\cdot(0.274)^2+2\cdot(0.064)^2+2\cdot(-0.330)^2+2\cdot(-0.232)^2+2\cdot(0.123)^2+2\cdot(0.341)^2+(0.182)^2+(-0.126)^2 \text{ solve, } q_6 \rightarrow .98411$$

$$q_7=2\cdot(0.330)^2+2\cdot(0.131)^2+2\cdot(0.231)^2+2\cdot(0.307)^2+2\cdot(0.062)^2+2\cdot(0.341)^2+2\cdot(0.125)^2+(0.273)^2+(-0.542)^2 \text{ solve, } q_7 \rightarrow 1.041555$$

$$q_8=2\cdot(0.342)^2+2\cdot(0.064)^2+2\cdot(-0.330)^2+2\cdot(-0.125)^2+2\cdot(0.308)^2+2\cdot(0.182)^2+2\cdot(0.273)^2+(0.228)^2+(-0.178)^2 \text{ solve, } q_8 \rightarrow .979872$$

$$q_9=2\cdot(0.342)^2+2\cdot(0.2623)^2+2\cdot(0.330)^2+2\cdot(0.123)^2+2\cdot(0.308)^2+2\cdot(-0.179)^2+2\cdot(0.275)^2+(0.229)^2+(-0.183)^2 \text{ solve, } q_9 \rightarrow .98073858$$

$$q_{10}=2\cdot(0.330)^2+2\cdot(-0.180)^2+2\cdot(0.232)^2+2\cdot(0.306)^2+2\cdot(0.065)^2+2\cdot(-0.342)^2+2\cdot(0.125)^2+(-0.275)^2+(0.341)^2 \text{ solve, } q_{10} \rightarrow 1.043054$$

$$q_{11}=2\cdot(0.274)^2+2\cdot(-0.273)^2+2\cdot(-0.064)^2+2\cdot(0.330)^2+2\cdot(-0.238)^2+2\cdot(-0.186)^2+2\cdot(0.342)^2+(-0.178)^2+(-0.12)^2 \text{ solve, } q_{11} \rightarrow .987694$$

$$q_{12}=2\cdot(0.231)^2+2\cdot(-0.330)^2+2\cdot(0.193)^2+2\cdot(0.182)^2+2\cdot(-0.342)^2+2\cdot(0.229)^2+2\cdot(0.066)^2+(0.308)^2+(-0.234)^2 \text{ solve, } q_{12} \rightarrow .96241$$

$$q_{13}=2\cdot(-0.342)^2+2\cdot(0.231)^2+2\cdot(0.273)^2+2\cdot(-0.062)^2+2\cdot(-0.182)^2+2\cdot(0.533)^2+2\cdot(-0.330)^2+(0.121)^2+(-0.329)^2 \text{ solve, } q_{13} \rightarrow 1.09292$$

$$q_{14}=2\cdot(0.182)^2+2\cdot(-0.307)^2+2\cdot(0.341)^2+2\cdot(0.273)^2+2\cdot(0.122)^2+2\cdot(0.065)^2+2\cdot(-0.233)^2+(0.331)^2+(-0.058)^2 \text{ solve, } q_{14} \rightarrow .896349$$

$$q_{15}=2\cdot(0.124)^2+2\cdot(-0.232)^2+2\cdot(0.308)^2+2\cdot(-0.342)^2+2\cdot(0.329)^2+2\cdot(-0.273)^2+2\cdot(0.18)^2+(0.06)^2+(-0.277)^2 \text{ solve, } q_{15} \rightarrow 1.072725$$

$$q_{16}=2\cdot(0.063)^2+2\cdot(-0.125)^2+2\cdot(0.182)^2+2\cdot(-0.233)^2+2\cdot(0.275)^2+2\cdot(-0.308)^2+2\cdot(0.331)^2+(0.342)^2+(0.342)^2 \text{ solve, } q_{16} \rightarrow .9332494$$

- Orde ikatan

$$P_{12}=2(0.063-0.124)+2(0.124-0.231)+2(0.182-0.308)+2(0.231-0.342)+2(0.274-0.342)+2(0.307-0.330)+2(0.350-0.274)+2(0.350-0.181)+1(0.342-0.064)+1(0.274-0.273) \rightarrow P_{12}=7.5865$$

$$P_{23}=2(0.181-0.124)+2(0.307-0.231)+2(0.341-0.308)+2(0.274-0.342)+2(0.124-0.330)+2(-0.064-0.274)+2(0.231-0.181)+1(-0.330-0.064)+1(-0.273-0.064) \rightarrow P_{23}=7.10936$$

$$P_{27}=2(-0.330-0.124)+2(0.181-0.231)+2(-0.231-0.308)+2(0.307-0.342)+2(0.062-0.330)+2(0.341-0.274)+2(0.125-0.181)+1(0.273-0.064)+1(-0.273-0.342) \rightarrow P_{27}=-430298$$

$$P_{34}=2(0.181-0.231)+2(0.307-0.342)+2(0.341-0.273)+2(0.274-0.342)+2(0.124-0.180)+2(-0.064-0.330)+2(0.231-0.307)+1(-0.330-0.125)+1(-0.064-0.330) \rightarrow P_{34}=674432$$

$$P_{45}=2(0.274-0.231)+2(0.330-0.242)+2(0.123-0.273)+2(-0.231-0.064)+2(-0.180-0.064)+2(-0.341-0.180)+2(-0.232-0.330)+2(0.062-0.307)+2(0.308-0.125)+1(0.330-0.230) \rightarrow P_{45}=595974$$

$$P_{55}=2(0.274-0.307)+2(0.333-0.274)+2(0.123-0.064)+2(-0.180-0.330)+2(-0.341-0.232)+2(-0.233-0.123)+2(0.062-0.341)+1(0.308-0.182)+1(-0.230-0.126) \rightarrow P_{56}=620204$$

$$P_{67}=2(0.330-0.307)+2(0.181-0.274)+2(-0.231-0.064)+2(-0.307-0.330)+2(0.062-0.232)+2(0.341-0.125)+2(0.125-0.341)+1(-0.273-0.182)+1(-0.125-0.242) \rightarrow P_{67}=5815956$$

$$P_{58}=2(0.274-0.342)+2(0.330-0.554)+2(0.123-0.330)+2(-0.180-0.125)+2(-0.341-0.305)+2(-0.341-0.125)+2(0.062-0.273)+2(0.662-0.273)+1(0.308-0.223)+1(-0.230-0.175) \rightarrow P_{58}=643612$$

$$P_{89}=2(0.344-0.342)+2(0.062-0.064)+2(-0.330-0.330)+2(0.123-0.125)+2(0.308-0.306)+2(-0.179-0.132)+2(-0.275-0.273)+1(0.229-0.223)+1(-0.178-0.183) \rightarrow P_{89}=485745$$

$$P_{910}=2(0.342-0.350)+2(0.062-0.181)+2(-0.330-0.232)+2(0.123-0.306)+2(0.308-0.065)+2(-0.179-0.342)+2(-0.275-0.122)+1(0.229-0.275)+1(0.341-0.183) \rightarrow P_{910}=52762$$

$$P_{914}=2(0.342-0.181)+2(0.062-0.307)+2(-0.330-0.341)+2(0.123-0.273)+2(0.308-0.122)+2(-0.179-0.066)+2(-0.275-0.233)+1(-0.229-0.331)+1(-0.183-0.058) \rightarrow P_{914}=720177$$

$$P_{1011}=2(0.307-0.330)+2(-0.273-0.181)+2(-0.064-0.232)+2(-0.330-0.306)+2(-0.230-0.065)+2(-0.126-0.342)+2(-0.234-0.122)+1(-0.178-0.275)+1(-0.341-0.12) \rightarrow P_{1011}=582864$$

$$P_{1112}=2(0.307-0.274)+2(-0.273-0.330)+2(-0.064-0.123)+2(0.330-0.182)+2(-0.230-0.342)+2(-0.125-0.229)+2(0.342-0.065)+1(-0.178-0.308)+1(-0.234-0.12) \rightarrow P_{1112}=590164$$

$$P_{1213}=2(0.231-0.274)+2(-0.342-0.330)+2(0.273-0.123)+2(-0.051-0.182)+2(-0.182-0.342)+2(0.331-0.229)+2(0.306-0.066)+1(0.121-0.308)+1(-0.234-0.329) \rightarrow P_{1213}=518702$$

$$P_{1314}=2(0.231-0.181)+2(-0.342-0.307)+2(-0.273-0.341)+2(-0.061-0.275)+2(-0.182-0.122)+2(0.331-0.066)+2(0.306-0.233)+1(0.121-0.331)+1(-0.329-0.058) \rightarrow P_{1314}=-588567$$

$$P_{1415}=2(-0.124-0.181)+2(-0.232-0.307)+2(0.308-0.341)+2(-0.342-0.273)+2(-0.329-0.122)+2(-0.272-0.065)+2(0.178-0.233)+1(-0.059-0.331)+1(-0.058-0.277) \rightarrow P_{1415}=.690013$$

$$P_{1516}=2(-0.124-0.063)+2(-0.232-0.125)+2(0.308-0.182)+2(-0.342-0.233)+2(-0.329-0.275)+2(-0.272-0.303)+2(0.178-0.331)+1(-0.059-0.342)+1(-0.277-0.304) \rightarrow P_{1516}=38458$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.759 \text{ solve}, F_1 \rightarrow .9730508075688772935$$

$$F_2 = \sqrt{3} - 0.759 - 0.710 - 0.430 \text{ solve}, F_2 \rightarrow -.1669491924311227065$$

$$F_3 = \sqrt{3} - 0.710 - 0.674 \text{ solve}, F_3 \rightarrow .3480508075688772935$$

$$F_4 = \sqrt{3} - 0.674 - 0.596 \text{ solve}, F_4 \rightarrow .4620508075688772935$$

$$F_5 = \sqrt{3} - 0.596 - 0.596 - - 0.044 \text{ solve}, F_5 \rightarrow .5840508075688772935$$

$$F_6 = \sqrt{3} - 0.596 - 0.582 \text{ solve}, F_6 \rightarrow .5540508075688772935$$

$$F_7 = \sqrt{3} - 0.430 - 0.582 \text{ solve}, F_7 \rightarrow .7200508075688772935$$

$$F_8 = \sqrt{3} - - 0.044 - 0.486 \text{ solve}, F_8 \rightarrow 1.2900508075688772935$$

$$F_9 = \sqrt{3} - 0.486 - 0.528 - 0.720 \text{ solve}, F_9 \rightarrow -.0019491924311227065000$$

$$F_{10} = \sqrt{3} - 0.528 - 0.533 \text{ solve}, F_{10} \rightarrow .6710508075688772935$$

$$F_{11} = \sqrt{3} - 0.533 - 0.590 \text{ solve}, F_{11} \rightarrow .6090508075688772935$$

$$F_{12} = \sqrt{3} - 0.590 - 0.519 \text{ solve}, F_{12} \rightarrow .6230508075688772935$$

$$F_{13} = \sqrt{3} - 0.519 - 0.586 \text{ solve}, F_{13} \rightarrow .6270508075688772935$$

$$F_{14} = \sqrt{3} - 0.720 - 0.589 - 0.690 \text{ solve}, F_{14} \rightarrow -.2669491924311227065$$

$$F_{15} = \sqrt{3} - 0.690 - 0.885 \text{ solve}, F_{15} \rightarrow .1570508075688772935$$

$$F_{16} = \sqrt{3} - 0.885 \text{ solve}, F_{16} \rightarrow .8470508075688772935$$

**D. 1 elektron tereksitasi ke 4 tingkat energi lebih tinggi**  
**-Kerapatan elektron { q }**

$$\begin{aligned}
 q_1 &= 2(0.063)^2 + 2(0.124)^2 + 2(0.181)^2 + 2(0.231)^2 + 2(0.274)^2 + 2(0.307)^2 + 2(0.330)^2 + (0.342)^2 + (0.231)^2 \text{ solve, } q_1 \rightarrow 0.957769 \\
 q_2 &= 2(0.124)^2 + 2(0.231)^2 + 2(0.307)^2 + 2(0.342)^2 + 2(0.330)^2 + 2(0.274)^2 + 2(0.181)^2 + (0.064)^2 + (-0.330)^2 \text{ solve, } q_2 \rightarrow 1.10657 \\
 q_3 &= 2(0.182)^2 + 2(0.308)^2 + 2(0.341)^2 + 2(0.273)^2 + 2(0.123)^2 + 2(-0.064)^2 + 2(-0.231)^2 + (-0.231)^2 + (0.123)^2 \text{ solve, } q_3 \rightarrow 206777 \\
 q_4 &= 2(0.231)^2 + 2(0.342)^2 + 2(0.274)^2 + 2(0.064)^2 + 2(-0.330)^2 + 2(-0.307)^2 + (-0.125)^2 + (0.182)^2 \text{ solve, } q_4 \rightarrow 1.018341 \\
 q_5 &= 2(0.274)^2 + 2(0.330)^2 + 2(0.124)^2 + 2(-0.180)^2 + 2(0.180)^2 + 2(0.330)^2 + 2(0.307)^2 + (-0.125)^2 + (0.182)^2 \text{ solve, } q_5 \rightarrow 1.022506 \\
 q_6 &= 2(0.367)^2 + 2(0.274)^2 + 2(-0.064)^2 + 2(-0.330)^2 + 2(-0.232)^2 + 2(0.123)^2 + 2(0.341)^2 + (0.182)^2 + (0.229)^2 \text{ solve, } q_6 \rightarrow 1.020675 \\
 q_7 &= 2(0.330)^2 + 2(0.131)^2 + 2(0.231)^2 + 2(0.307)^2 + 2(0.062)^2 + 2(0.341)^2 + 2(0.123)^2 + (0.273)^2 + (0.065)^2 \text{ solve, } q_7 \rightarrow 0.928927 \\
 q_8 &= 2(0.342)^2 + 2(0.064)^2 + 2(-0.330)^2 + 2(-0.125)^2 + 2(0.308)^2 + 2(0.182)^2 + 2(-0.273)^2 + (0.223)^2 + (0.303)^2 \text{ solve, } q_8 \rightarrow 1.043052 \\
 q_9 &= 2(0.342)^2 + 2(0.0623)^2 + 2(-0.330)^2 + 2(0.123)^2 + 2(0.398)^2 + 2(-0.179)^2 + 2(-0.275)^2 + (0.225)^2 + (0.305)^2 \text{ solve, } q_9 \rightarrow 1.04021453 \\
 q_{10} &= 2(0.330)^2 + 2(-0.180)^2 + 2(-0.232)^2 + 2(0.306)^2 + 2(0.065)^2 + 2(-0.342)^2 + 2(0.125)^2 + (-0.275)^2 + (-0.059)^2 \text{ solve, } q_{10} \rightarrow 0.930254 \\
 q_{11} &= 2(0.274)^2 + 2(-0.273)^2 + 2(-0.064)^2 + 2(0.330)^2 + 2(-0.238)^2 + 2(-0.186)^2 + 2(-0.342)^2 + (-0.173)^2 + (-0.234)^2 \text{ solve, } q_{11} \rightarrow 1.028305 \\
 q_{12} &= 2(0.231)^2 + 2(-0.330)^2 + 2(0.193)^2 + 2(0.182)^2 + 2(-0.342)^2 + 2(-0.229)^2 + 2(0.066)^2 + (0.303)^2 + (0.341)^2 \text{ solve, } q_{12} \rightarrow 1.023935 \\
 q_{13} &= 2(-0.342)^2 + 2(0.231)^2 + 2(0.273)^2 + 2(-0.062)^2 + 2(-0.182)^2 + 2(-0.331)^2 + 2(-0.306)^2 + (0.121)^2 + (-0.176)^2 \text{ solve, } q_{13} \rightarrow 1.015655 \\
 q_{14} &= 2(0.182)^2 + 2(-0.307)^2 + 2(0.341)^2 + 2(0.273)^2 + 2(0.122)^2 + 2(0.066)^2 + 2(-0.233)^2 + (-0.129)^2 \text{ solve, } q_{14} \rightarrow 0.909626 \\
 q_{15} &= 2(0.124)^2 + 2(-0.232)^2 + 2(0.308)^2 + 2(-0.342)^2 + 2(0.329)^2 + 2(-0.273)^2 + 2(0.18)^2 + (0.06)^2 + (0.331)^2 \text{ solve, } q_{15} \rightarrow 1.105557 \\
 q_{16} &= 2(0.063)^2 + 2(-0.125)^2 + 2(0.182)^2 + 2(-0.233)^2 + 2(0.275)^2 + 2(-0.308)^2 + 2(0.331)^2 + (0.222)^2 + (-0.270)^2 \text{ solve, } q_{16} \rightarrow 0.963978
 \end{aligned}$$

### - Orde ikatan

$$P_{12}=2(-0.063-0.124)+2-(0.124-0.231)+2-(0.182-0.308)+2-(0.231-0.342)+2-(0.274-0.330)+2-(0.307-0.274)+2-(0.330-0.181)+1-(0.242-0.064)+1-(0.231-0.330) \rightarrow P_{12}=7.57222$$

$$P_{23}=2(0.181-0.124)+2-(0.307-0.231)+2-(0.341-0.308)+2-(0.274-0.342)+2-(0.124-0.330)+2-(0.064-0.274)+2-(0.231-0.181)+1-(0.330-0.064)+1-(0.330-0.123) \rightarrow P_{23}=6.52874$$

$$P_{27}=2(-0.330-0.124)+2-(0.181-0.231)+2(-0.231-0.308)+2-(0.307-0.342)+2-(0.052-0.330)+2-(0.341-0.274)+2-(0.125-0.181)+1-(0.273-0.066)+1-(0.350-0.066) \rightarrow P_{27}=5.54444$$

$$P_{34}=2(0.181-0.231)+2-(0.307-0.342)+2-(0.341-0.273)+2-(0.274-0.064)+2-(0.124-0.180)+2-(0.064-0.330)+2-(0.231-0.307)+1-(0.330-0.125)+1-(0.123-0.182) \rightarrow P_{34}=7.17958$$

$$P_{45}=2(0.274-0.231)+2-(0.330-0.342)+2-(0.123-0.273)+2(-0.341-0.180)+2(-0.232-0.330)+2-(0.062-0.307)+1-(0.303-0.125)+1-(0.182-0.342) \rightarrow P_{45}=6.09623$$

$$P_{56}=2(0.274-0.307)+2-(0.330-0.274)+2-(0.123-0.064)+2(-0.180-0.330)+2(-0.231-0.064)+2(-0.341-0.232)+2-(0.123-0.123)+2-(0.062-0.341)+1-(0.308-0.182)+1-(0.342-0.229) \rightarrow P_{56}=5.73386$$

$$P_{67}=2(0.330-0.307)+2-(0.181-0.274)+2(-0.231-0.064)+2(-0.367-0.330)+2-(0.062-0.232)+2-(0.341-0.123)+2-(0.125-0.341)+1-(0.273-0.182)+1-(0.229-0.066) \rightarrow P_{67}=6.39792$$

$$P_{73}=2(0.274-0.342)+2-(0.330-0.624)+2-(0.123-0.330)+2(-0.180-0.125)+2(-0.341-0.306)+2(-0.232-0.182)+2-(0.062-0.273)+1-(0.308-0.223)+1-(0.342-0.308) \rightarrow P_{73}=10.2464$$

$$P_{89}=2(0.342-0.342)+2-(0.062-0.064)+2(-0.330-0.330)+2-(0.123-0.125)+2-(0.308-0.306)+2(-0.179-0.182)+2(-0.275-0.273)+1-(0.229-0.223)+1-(0.308-0.305) \rightarrow P_{89}=5.47111$$

$$P_{910}=2(0.342-0.330)+2-(0.062-0.181)+2(-0.330-0.232)+2-(0.123-0.305)+2-(0.308-0.065)+2(-0.179-0.342)+2(-0.275-0.122)+1-(0.229-0.275)+1-(0.305-0.059) \rightarrow P_{910}=6.03018$$

$$P_{914}=2(0.342-0.181)+2-(0.062-0.307)+2(-0.330-0.341)+2-(0.123-0.273)+2-(0.308-0.122)+2(-0.179-0.566)+2(-0.275-0.233)+1-(0.229-0.331)+1-(0.305-0.129) \rightarrow P_{914}=6.70218$$

$$P_{1011}=2(0.307-0.350)+2(-0.273-0.181)+2(-0.064-0.232)+2-(0.330-0.306)+2(-0.230-0.065)+2(-0.126-0.342)+2-(0.242-0.122)+1-(0.059-0.234) \rightarrow P_{1011}=6.10078$$

$$P_{1112}=2(0.307-0.274)+2(-0.273-0.330)+2(-0.064-0.123)+2(0.330-0.182)+2(-0.230-0.342)+2(-0.125-0.229)+2-(0.342-0.066)+1-(0.234-0.341) \rightarrow P_{1112}=4.82229$$

$$P_{1213}=2(0.231-0.274)+2(-0.342-0.330)+2(-0.061-0.182)+2(-0.273-0.123)+2(-0.182-0.342)+2(0.331-0.229)+2(0.306-0.065)+1-(0.121-0.308)+1-(0.341-0.176) \rightarrow P_{1213}=5.35672$$

$$P_{1314}=2(0.223-0.181)+2(-0.342-0.307)+2(0.273-0.341)+2(-0.061-0.273)+2(-0.182-0.122)+2(0.331-0.066)+2(0.305-0.233)+1-(0.121-0.331)+1-(0.234-0.341) \rightarrow P_{1314}=6.30353$$

$$P_{1415}=2(-0.124-0.181)+2(-0.222-0.307)+2(0.308-0.341)+2(-0.342-0.273)+2(0.329-0.122)+2(-0.272-0.066)+2(0.178-0.233)+1(-0.059-0.331)+1(-0.129-0.331) \rightarrow P_{1415}=6.31248$$

$$P_{1516}=2(-0.124-0.063)+2(-0.252-0.125)+2(0.308-0.182)+2(-0.342-0.233)+2(0.329-0.275)+2(-0.272-0.308)+2(0.178-0.331)+1(-0.059-0.342)+1(-0.129-0.331) \rightarrow P_{1516}=7.11006$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.757 \text{ solve}, F_1 \rightarrow .9750508075688772935$$

$$F_2 = \sqrt{3} - 0.757 - 0.653 - 0.545 \text{ solve}, F_2 \rightarrow -.2229491924311227065$$

$$F_3 = \sqrt{3} - 0.653 - 0.718 \text{ solve}, F_3 \rightarrow .3610508075688772935$$

$$F_4 = \sqrt{3} - 0.718 - 0.609 \text{ solve}, F_4 \rightarrow .4050508075688772935$$

$$F_5 = \sqrt{3} - 0.573 - 0.609 - 0.102 \text{ solve}, F_5 \rightarrow .6520508075688772935$$

$$F_6 = \sqrt{3} - 0.573 - 0.639 \text{ solve}, F_6 \rightarrow .5200508075688772935$$

$$F_7 = \sqrt{3} - 0.545 - 0.639 \text{ solve}, F_7 \rightarrow .5480508075688772935$$

$$F_8 = \sqrt{3} - 0.102 - 0.547 \text{ solve}, F_8 \rightarrow 1.2870508075688772935$$

$$F_9 = \sqrt{3} - 0.547 - 0.608 - 0.670 \text{ solve}, F_9 \rightarrow -.092949192431122706500$$

$$F_{10} = \sqrt{3} - 0.608 - 0.610 \text{ solve}, F_{10} \rightarrow .5140508075688772935$$

$$F_{11} = \sqrt{3} - 0.610 - 0.482 \text{ solve}, F_{11} \rightarrow .6400508075688772935$$

$$F_{12} = \sqrt{3} - 0.482 - 0.536 \text{ solve}, F_{12} \rightarrow .7140508075688772935$$

$$F_{13} = \sqrt{3} - 0.536 - 0.630 \text{ solve}, F_{13} \rightarrow .5660508075688772935$$

$$F_{14} = \sqrt{3} - 0.630 - 0.670 - 0.631 \text{ solve}, F_{14} \rightarrow -.1989491924311227065$$

$$F_{15} = \sqrt{3} - 0.631 - 0.711 \text{ solve}, F_{15} \rightarrow .3900508075688772935$$

$$F_{16} = \sqrt{3} - 0.711 \text{ solve}, F_{16} \rightarrow 1.0210508075688772935$$



### A.3. Fenolstalein dalam suasana basa (kromofor II)

x+2	0.9	0	0	0	0	0	0	0	0	0	0	0	0	- 2.53791753
0.9	x	1	0	0	0	1	0	0	0	0	0	0	0	- 2.53791753
0	1	x	1	0	0	0	0	0	0	0	0	0	0	- 1.54786166
0	0	1	x	1	0	0	0	0	0	0	0	0	0	- 1.29938751
0	0	0	1	x	1	0	1	0	0	0	0	0	0	- .804540882
0	0	0	0	1	x	1	0	0	0	0	0	0	0	- .804540882
0	0	0	0	0	1	x	1	0	0	0	0	0	0	- .395652236
0	1	0	0	0	1	x	0	0	0	0	0	0	0	.234688325
0	0	0	0	1	0	0	x	1	0	0	0	0	0	.234688325
0	0	0	0	0	0	1	x	1	0	0	0	1	0	1.14028304
0	0	0	0	0	0	0	1	x	1	0	0	0	0	1.14028304
0	0	0	0	0	0	0	0	1	x	1	0	0	0	1.42938751
0	0	0	0	0	0	0	0	0	1	x	1	0	1	1.42938751
0	0	0	0	0	0	0	0	0	0	1	x	1	0	2.00296916
0	0	0	0	0	0	0	0	0	0	0	1	0	0	2.00296916
0	0	0	0	0	0	0	0	0	0	0	0	1	0	x + 2

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} nm \cdot 6.023 \cdot 10^{23}}{(-39565223 - 2346883259) \cdot -25390 \cdot 4.18 \cdot \frac{J}{mol} \cdot \lambda} = \frac{sec \cdot mol}{\lambda}$$

solve,  $\lambda \rightarrow 604.281334 \text{ nm}$



## LAMPIRAN B

### HASIL PERHITUNGAN TEORI HMO UNTUK MOLEKUL METIL KUNING

DENGAN  $k_{CN} = 0.7$ ,  $h_H^t = 2$  DAN  $h_N = 1.5$

#### A.1. Metil kuning pada suasana basa

Perhitungan untuk mendapatkan panjang gelombang maksimum ( $\Delta E = E_{LUMO} - E_{HOMO}$ )

$x$	1	0	0	0	1	0	0	0	0	0	0	0	0	0	-3.587357	
1	$x$	1	0	0	0	0	0	0	0	0	0	0	0	0	-2.088195	
0	1	$x$	1	0	0	0	0	0	0	0	0	0	0	0	-2.088195	
0	0	1	$x$	1	0	0.7	0	0	0	0	0	0	0	0	-1.578666	
0	0	0	1	$x$	1	0	0	0	0	0	0	0	0	0	-1.578666	
1	0	0	0	1	$x$	0	0	0	0	0	0	0	0	0	-0.901208	
0	0	0	0.7	0	0	$x+1.5$	0.7	0	0	0	0	0	0	0	-0.271989	
0	0	0	0	0	0	0.7	$x+1.5$	0.7	0	0	0	0	0	0	solve, $x \rightarrow -0.238133$	
0	0	0	0	0	0	0	0.7	$x$	1	0	0	0	1	0	0.3990919	
0	0	0	0	0	0	0	0	1	$x$	1	0	0	0	0	0.6853610	
0	0	0	0	0	0	0	0	0	1	$x$	1	0	0	0	0.9012087	
0	0	0	0	0	0	0	0	0	0	1	$x$	1	0	0.7	1.3855896	
0	0	0	0	0	0	0	0	0	0	0	1	$x$	1	0	1.3855896	
0	0	0	0	0	0	0	0	1	0	0	0	1	$x$	0	1.9162144	
0	0	0	0	0	0	0	0	0	1	0	0	0	1	$x$	0	2.2093624

$$(-0.238133 - 0.3990919) \cdot 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot J \cdot \text{sec} \cdot 3 \cdot 10^{17} \text{ nm} \cdot 6.023 \cdot 10^{23}}{\text{sec} \cdot \text{mol} \cdot \lambda}$$

solve,  $\lambda \rightarrow 596.214358 \text{ nm}$

## a.2 Fungsi gelombang

$$\begin{aligned}\psi_1 &= 0.069\phi_1 + 0.135\phi_2 + 0.196\phi_3 + 0.250\phi_4 + 0.294\phi_5 + 0.327\phi_6 + 0.347\phi_7 + \\&\quad 0.354\phi_8 + 0.347\phi_9 + 0.327\phi_{10} + 0.294\phi_{11} + 0.250\phi_{12} + 0.196\phi_{13} + 0.135\phi_{14} + \\&\quad 0.069\phi_{15} \\ \psi_2 &= 0.135\phi_1 + 0.250\phi_2 + 0.327\phi_3 + 0.354\phi_4 + 0.327\phi_5 + 0.250\phi_6 + 0.135\phi_7 + 0\phi_8 - \\&\quad 0.135\phi_9 - 0.250\phi_{10} - 0.326\phi_{11} - 0.354\phi_{12} - 0.327\phi_{13} - 0.250\phi_{14} - 0.135\phi_{15} \\ \psi_3 &= 0.196\phi_1 + 0.327\phi_2 + 0.347\phi_3 + 0.250\phi_4 + 0.069\phi_5 - 0.135\phi_6 - 0.294\phi_7 - 0.354\phi_8 \\&\quad - 0.294\phi_9 - 0.136\phi_{10} + 0.068\phi_{11} + 0.249\phi_{12} + 0.346\phi_{13} + 0.327\phi_{14} + 0.198\phi_{15} \\ \psi_4 &= 0.250\phi_1 + 0.354\phi_2 + 0.250\phi_3 + 0\phi_4 - 0.254\phi_5 + 0.354\phi_6 - 0.250\phi_7 + 0\phi_8 + \\&\quad 0.249\phi_9 + 0.354\phi_{10} + 0.251\phi_{11} + 0\phi_{12} - 0.249\phi_{13} - 0.354\phi_{14} - 0.251\phi_{15} \\ \psi_5 &= 0.294\phi_1 + 0.327\phi_2 + 0.069\phi_3 + 0.250\phi_4 + 0.347\phi_5 - 0.135\phi_6 + 0.195\phi_7 + \\&\quad 0.354\phi_8 + 0.198\phi_9 - 0.134\phi_{10} - 0.346\phi_{11} - 0.251\phi_{12} + 0.067\phi_{13} + 0.326\phi_{14} + \\&\quad 0.295\phi_{15} \\ \psi_6 &= 0.327\phi_1 + 0.250\phi_2 - 0.135\phi_3 + 0.354\phi_4 + 0.135\phi_5 + 0.249\phi_6 + 0.327\phi_7 + 0\phi_8 - \\&\quad 0.326\phi_9 - 0.251\phi_{10} + 0.133\phi_{11} + 0.354\phi_{12} + 0.138\phi_{13} - 0.248\phi_{14} - 0.328\phi_{15} \\ \psi_7 &= 0.347\phi_1 + 0.136\phi_2 - 0.294\phi_3 - 0.251\phi_4 + 0.195\phi_5 + 0.327\phi_6 - 0.067\phi_7 - 0.354\phi_8 \\&\quad - 0.326\phi_9 - 0.251\phi_{10} + 0.133\phi_{11} + 0.354\phi_{12} + 0.138\phi_{13} - 0.248\phi_{14} - 0.328\phi_{15} \\ \psi_8 &= 0.354\phi_1 + 0\phi_2 - 0.354\phi_3 + 0\phi_4 + 0.354\phi_5 + 0\phi_6 - 0.354\phi_7 + 0\phi_8 + 0.354\phi_9 - 0\phi_{10} \\&\quad - 0.354\phi_{11} + 0\phi_{12} + 0.354\phi_{13} - 0\phi_{14} - 0.354\phi_{15} \\ \psi_9 &= 0.347\phi_1 - 0.135\phi_2 - 0.294\phi_3 + 0.249\phi_4 + 0.198\phi_5 + 0.326\phi_6 - 0.069\phi_7 + 0.354\phi_8 \\&\quad - 0.066 - 0.328\phi_{10} + 0.194\phi_{11} + 0.253\phi_{12} - 0.292\phi_{13} - 0.139\phi_{14} - 0.346\phi_{15} \\ \psi_{10} &= 0.327\phi_1 - 0.250\phi_2 - 0.136\phi_3 + 0.354\phi_4 - 0.134\phi_5 - 0.250\phi_6 + 0.326\phi_7 - 0\phi_8 - \\&\quad 0.328\phi_9 + 0.247\phi_{10} + 0.135\phi_{11} - 0.354\phi_{12} + 0.131\phi_{13} + 0.250\phi_{14} - 0.325\phi_{15} \\ \psi_{11} &= 0.294\phi_1 - 0.326\phi_2 + 0.068\phi_3 + 0.250\phi_4 - 0.346\phi_5 + 0.133\phi_6 + 0.196\phi_7 - 0.354\phi_8 \\&\quad + 0.196\phi_9 + 0.135\phi_{10} - 0.348\phi_{11} + 0.50\phi_{12} + 0.069\phi_{13} - 0.329\phi_{14} + 0.294\phi_{15} \\ \psi_{12} &= 0.250\phi_1 - 0.354\phi_2 + 0.294\phi_3 - 0\phi_4 - 0.251\phi_5 + 0.354\phi_6 - 0.248\phi_7 - 0\phi_8 + \\&\quad 0.253\phi_9 - 0.354\phi_{10} + 0.247\phi_{11} + 0.005\phi_{12} - 0.254\phi_{13} + 0.354\phi_{14} - 0.245\phi_{15} \\ \psi_{13} &= 0.197\phi_1 - 0.327\phi_2 + 0.346\phi_3 - 0.249\phi_4 + 0.067\phi_5 + 0.138\phi_6 - 0.296\phi_7 + 0.350\phi_8 \\&\quad - 0.292\phi_9 + 0.131\phi_{10} + 0.074\phi_{11} - 0.254\phi_{12} + 0.348\phi_{13} - 0.324\phi_{14} + 0.191\phi_{15} \\ \psi_{14} &= 0.136\phi_1 - 0.251\phi_2 + 0.327\phi_3 - 0.354\phi_4 + 0.326\phi_5 - 0.248\phi_6 + 0.132\phi_7 - 0\phi_8 - \\&\quad 0.139\phi_9 + 0.253\phi_{10} - 0.329\phi_{11} + 0.354\phi_{12} - 0.324\phi_{13} + 0.245\phi_{14} - 0.128\phi_{15} \\ \psi_{15} &= 0.069\phi_1 - 0.136\phi_2 + 0.198\phi_3 - 0.251\phi_4 + 0.295\phi_5 - 0.328\phi_6 + 0.347\phi_7 - 0.354\phi_8 \\&\quad + 0.346\phi_9 - 0.325\phi_{10} + 0.291\phi_{11} - 0.254\phi_{12} + 0.191\phi_{13} - 0.128\phi_{14} + 0.061\phi_{15} \end{aligned}$$

### a.3 Indeks keraktifan

#### - Kerapatan Elektron

$$\begin{aligned}q_1 &= 2 \cdot (0.069)^2 + 2 \cdot (0.135)^2 + 2 \cdot (0.196)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0.294)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0.347)^2 + 2 \cdot (0.354)^2 \text{ solve, } q_1 \rightarrow 1.125984 \\q_2 &= 2 \cdot (0.135)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0.354)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0.135)^2 + 2 \cdot (0)^2 \text{ solve, } q_2 \rightarrow 1.001248 \\q_3 &= 2 \cdot (0.196)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0.347)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0.069)^2 + 2 \cdot (-0.135)^2 + 2 \cdot (-0.294)^2 + 2 \cdot (-0.354)^2 \text{ solve, } q_3 \rightarrow 1.125984 \\q_4 &= 2 \cdot (0.250)^2 + 2 \cdot (0.354)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.254)^2 + 2 \cdot (0.354)^2 + 2 \cdot (-0.250)^2 + 2 \cdot (0)^2 \text{ solve, } q_4 \rightarrow 1.005296 \\q_5 &= 2 \cdot (0.294)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0.069)^2 + 2 \cdot (0.250)^2 + 2 \cdot (0.347)^2 + 2 \cdot (-0.135)^2 + 2 \cdot (0.195)^2 + 2 \cdot (0.354)^2 \text{ solve, } q_5 \rightarrow 1.125202 \\q_6 &= 2 \cdot (0.327)^2 + 2 \cdot (0.250)^2 + 2 \cdot (-0.135)^2 + 2 \cdot (0.354)^2 + 2 \cdot (0.135)^2 + 2 \cdot (0.249)^2 + 2 \cdot (0.327)^2 + 2 \cdot (0)^2 \text{ solve, } q_6 \rightarrow 1.00025 \\q_7 &= 2 \cdot (0.347)^2 + 2 \cdot (0.136)^2 + 2 \cdot (-0.291)^2 + 2 \cdot (-0.251)^2 + 2 \cdot (0.195)^2 + 2 \cdot (0.327)^2 + 2 \cdot (-0.067)^2 + 2 \cdot (-0.354)^2 \text{ solve, } q_7 \rightarrow 1.122692 \\q_8 &= 2 \cdot (0.354)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.354)^2 + 2 \cdot (0)^2 + 2 \cdot (0.354)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.354)^2 + 2 \cdot (0)^2 \text{ solve, } q_8 \rightarrow 1.002528 \\q_9 &= 2 \cdot (0.347)^2 + 2 \cdot (-0.135)^2 + 2 \cdot (-0.294)^2 + 2 \cdot (0.294)^2 + 2 \cdot (0.198)^2 + 2 \cdot (0.326)^2 + 2 \cdot (-0.069)^2 + 2 \cdot (0.354)^2 \text{ solve, } q_9 \rightarrow 1.174126 \\q_{10} &= 2 \cdot (0.327)^2 + 2 \cdot (-0.250)^2 + 2 \cdot (-0.136)^2 + 2 \cdot (0.354)^2 + 2 \cdot (-0.134)^2 + 2 \cdot (-0.250)^2 + 2 \cdot (0)^2 \text{ solve, } q_{10} \rightarrow .999946 \\q_{11} &= 2 \cdot (0.294)^2 + 2 \cdot (-0.326)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.250)^2 + 2 \cdot (-0.346)^2 + 2 \cdot (0.133)^2 + 2 \cdot (0.196)^2 + 2 \cdot (-0.354)^2 \text{ solve, } q_{11} \rightarrow 1.121946 \\q_{12} &= 2 \cdot (0.250)^2 + 2 \cdot (-0.354)^2 + 2 \cdot (0.249)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.251)^2 + 2 \cdot (0.354)^2 + 2 \cdot (-0.248)^2 + 2 \cdot (0)^2 \text{ solve, } q_{12} \rightarrow .999276 \\q_{13} &= 2 \cdot (0.197)^2 + 2 \cdot (-0.327)^2 + 2 \cdot (0.346)^2 + 2 \cdot (-0.249)^2 + 2 \cdot (0.067)^2 + 2 \cdot (0.138)^2 + 2 \cdot (0.350)^2 + 2 \cdot (0.350)^2 \text{ solve, } q_{13} \rightarrow 1.122208 \\q_{14} &= 2 \cdot (0.136)^2 + 2 \cdot (-0.251)^2 + 2 \cdot (0.327)^2 + 2 \cdot (-0.354)^2 + 2 \cdot (0.327)^2 + 2 \cdot (-0.248)^2 + 2 \cdot (0.132)^2 + 2 \cdot (0)^2 \text{ solve, } q_{14} \rightarrow .999198 \\q_{15} &= 2 \cdot (0.069)^2 + 2 \cdot (-0.136)^2 + 2 \cdot (0.198)^2 + 2 \cdot (-0.251)^2 + 2 \cdot (0.295)^2 + 2 \cdot (-0.328)^2 + 2 \cdot (-0.347)^2 + 2 \cdot (-0.354)^2 \text{ solve, } q_{15} \rightarrow 1.131592\end{aligned}$$

**\* Orde ikatan**

$$P_{12}=2\{-0.069-0.135\}+2\{-0.135-0.250\}+2\{-0.195-0.327\}+2\{-0.250-0.354\}+2\{-0.294-0.327\}+2\{-0.327-0.250\}+2\{-0.347-0.136\}+2\{-0.354-0\} \rightarrow P_{12}=841474$$

$$P_{16}=2\{-0.069-0.327\}+2\{-0.135-0.250\}+2\{-0.195-0.135\}+2\{-0.250-0.354\}+2\{-0.294-0.135\}+2\{-0.327-0.249\}+2\{-0.347-0.327\}+2\{-0.354-0\} \rightarrow P_{16}=54711$$

$$P_{23}=2\{-0.196-0.135\}+2\{-0.327-0.250\}+2\{-0.347-0.327\}+2\{-0.250-0.354\}+2\{-0.069-0.327\}+2\{-0.135-0.250\}+2\{-0.347-0.136\}+2\{-0.354-0\} \rightarrow P_{23}=518016$$

$$P_{24}=2\{-0.196-0.250\}+2\{-0.327-0.354\}+2\{-0.347-0.250\}+2\{-0.250-0\}+2\{-0.069-0.250\}+2\{-0.135-0.354\}+2\{-0.294-0.251\}+2\{-0.354-0\} \rightarrow P_{24}=538524$$

$$P_{45}=2\{-0.294-0.250\}+2\{-0.327-0.354\}+2\{-0.069-0.250\}+2\{-0.254-0\}+2\{-0.347-0.250\}+2\{-0.135-0.354\}+2\{-0.195-0.251\}+2\{-0.354-0\} \rightarrow P_{45}=534266$$

$$P_{47}=2\{-0.347-0.250\}+2\{-0.135-0.354\}+2\{-0.294-0.250\}+2\{-0.250-0\}+2\{-0.195-0.250\}+2\{-0.347-0.354\}+2\{-0.067-0.251\}+2\{-0.354-0\} \rightarrow P_{47}=48473$$

$$P_{55}=2\{-0.294-0.327\}+2\{-0.327-0.250\}+2\{-0.069-0.135\}+2\{-0.254-0.354\}+2\{-0.347-0.135\}+2\{-0.135-0.249\}+2\{-0.195-0.327\}+2\{-0.354-0\} \rightarrow P_{55}=670368$$

$$P_{78}=2\{-0.347-0.354\}+2\{-0.135-0\}+2\{-0.294-0.345\}+2\{-0.250-0\}+2\{-0.195-0.354\}+2\{-0.327-0\}+2\{-0.067-0.354\}+2\{-0.354-0\} \rightarrow P_{78}=634032$$

$$P_{89}=2\{-0.347-0.354\}+2\{-0.135-0\}+2\{-0.294-0.345\}+2\{-0.249-0\}+2\{-0.198-0.354\}+2\{-0.326-0.354\}+2\{-0.326-0.251\}+2\{-0.354-0\} \rightarrow P_{89}=819528$$

$$P_{910}=2\{-0.347-0.327\}+2\{-0.135-0.250\}+2\{-0.294-0.250\}+2\{-0.294-0.136\}+2\{-0.249-0.354\}+2\{-0.249-0.134\}+2\{-0.198-0.134\}+2\{-0.326-0.251\}+2\{-0.354-0\} \rightarrow P_{910}=497634$$

$$P_{914}=2\{-0.294-0.135\}+2\{-0.135-0.250\}+2\{-0.294-0.327\}+2\{-0.249-0.327\}+2\{-0.198-0.326\}+2\{-0.326-0.248\}+2\{-0.354-0\} \rightarrow P_{914}=629662$$

$$P_{1011}=2\{-0.294-0.327\}+2\{-0.326-0.250\}+2\{-0.068-0.136\}+2\{-0.251-0.354\}+2\{-0.246-0.134\}+2\{-0.133-0.251\}+2\{-0.193-0.251\}+2\{-0.354-0\} \rightarrow P_{1011}=473624$$

$$P_{1112}=2\{-0.294-0.250\}+2\{-0.326-0.354\}+2\{-0.068-0.249\}+2\{-0.251-0\}+2\{-0.346-0.251\}+2\{-0.133-0.354\}+2\{-0.133-0.354\}+2\{-0.354-0\} \rightarrow P_{1112}=773692$$

$$P_{1213}=2\{-0.196-0.250\}+2\{-0.327-0.354\}+2\{-0.346-0.249\}+2\{-0.249-0\}+2\{-0.067-0.251\}+2\{-0.138-0.354\}+2\{-0.138-0.354\}+2\{-0.354-0\} \rightarrow P_{1213}=663598$$

$$P_{1215}=2\{-0.069-0.250\}+2\{-0.135-0.354\}+2\{-0.198-0.249\}+2\{-0.251-0\}+2\{-0.295-0.251\}+2\{-0.328-0.354\}+2\{-0.328-0.354\}+2\{-0.354-0\} \rightarrow P_{1215}=841222$$

$$P_{1314}=2\{-0.196-0.135\}+2\{-0.327-0.220\}+2\{-0.346-0.327\}+2\{-0.249-0.354\}+2\{-0.087-0.326\}+2\{-0.138-0.248\}+2\{-0.138-0.248\}+2\{-0.354-0\} \rightarrow P_{1314}=5225784$$

- Harga valensi bebas

$$F_r \approx N_{\max} \sim N_r$$

$$F_1 = \sqrt{3} - 0.841 - 0.547 \text{ solve } F_1 \rightarrow .3440508075688772935$$

$$F_2 = \sqrt{3} - 0.841 - 0.518 \text{ solve } F_2 \rightarrow .3730508075688772935$$

$$F_3 = \sqrt{3} - 0.518 - 0.589 \text{ solve } F_3 \rightarrow .6250508075688772935$$

$$F_4 = \sqrt{3} - 0.589 - 0.584 - 0.485 \text{ solve } F_4 \rightarrow .074050807568877293500$$

$$F_5 = \sqrt{3} - 0.583 - 0.485 \text{ solve } F_5 \rightarrow .6640508075688772935$$

$$F_6 = \sqrt{3} - 0.547 - 0.671 \text{ solve } F_6 \rightarrow .5140508075688772935$$

$$F_7 = \sqrt{3} - 0.485 - 0.634 \text{ solve } F_7 \rightarrow .6130508075688772935$$

$$F_8 = \sqrt{3} - 0.634 - 0.819 \text{ solve } F_8 \rightarrow .2790508075688772935$$

$$F_9 = \sqrt{3} - 0.497 - 0.629 - 0.819 \text{ solve } F_9 \rightarrow -.2129491924311227065$$

$$F_{10} = \sqrt{3} - 0.497 - 0.474 \text{ solve } F_{10} \rightarrow .7610508075688772935$$

$$F_{11} = \sqrt{3} - 0.474 - 0.774 \text{ solve } F_{11} \rightarrow .4840508075688772935$$

$$F_{12} = \sqrt{3} - 0.774 - 0.663 - 0.841 \text{ solve } F_{12} \rightarrow -.5459491924311227065$$

$$F_{13} = \sqrt{3} - 0.663 - 0.525 \text{ solve } F_{13} \rightarrow .5440508075688772935$$

$$F_{14} = \sqrt{3} - 0.525 - 0.629 \text{ solve } F_{14} \rightarrow .5780508075688772935$$

$$F_{15} = \sqrt{3} - 0.841 \text{ solve } F_{15} \rightarrow .8910508075688772935$$

## B.2. Metil kuning pada suasana asam

Perhitungan untuk mendapatkan panjang gelombang maksimum ( $\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$ )

### a.1 $\lambda$ maksimum

[x 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0]	[-2.2341053712318578371]
[1 x 1 0 0 0 0 0 0 0 0 0 0 0 0 0]	[-2.1963919982533006419]
[0 1 x 1 0 0 0 0 0 0 0 0 0 0 0 0]	[-2.1963919982533006419]
[0 0 1 x 1 0 0.7 0 0 0 0 0 0 0 0 0]	[-1.1879138523511852661]
[0 0 0 1 x 1 0 0 0 0 0 0 0 0 0 0 0]	[-1.1879138523511852661]
[1 0 0 0 1 x 0 0 0 0 0 0 0 0 0 0 0]	[-83514078873266323477]
[0 0 0 0.7 0 0 x+1.5 0.7 0 0 0 0 0 0 0]	[-49847921020980169319]
[0 0 0 0 0 0 0.7 x+1.5 0.7 0 0 0 0 0 0]	[.04074699141130714908]
[0 0 0 0 0 0 0 0.7 x 1 0 0 0 0 0 0]	[.04074699141130714908]
[0 0 0 0 0 0 0 0 x 1 0 0 0 0 0 0]	[.83514078873266323477]
[0 0 0 0 0 0 0 0 0 x 1 0 0 0 0 0]	[1.1062050746158609955]
[0 0 0 0 0 0 0 0 0 0 x 1 0 0 0 0]	[1.1062050746158609955]
[0 0 0 0 0 0 0 0 0 0 0 x 1 x 1]	[2.0720639413290464216]
[0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 x]	[2.0720639413290464216]

solve ,x →

$$(-.49847921020980) - (.040746991411307) - 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot 3 \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\lambda}$$

solve , $\lambda \rightarrow 704.45365285156662516 \cdot \text{nm}$

### a.2. Fungsi gelombang

$$\begin{aligned}\psi_1 = & 0.051\phi_1 + 0.068\phi_2 + 0.131\phi_3 + 0.282\phi_4 + 0.131\phi_5 + 0.068\phi_6 + 0.612\phi_7 + \\& 0.612\phi_8 + 0.282\phi_9 + 0.131\phi_{10} + 0.068\phi_{11} + 0.051\phi_{12} + 0.068\phi_{13} + 0.131\phi_{14} \\\psi_2 = & 0.267\phi_1 + 0.273\phi_2 + 0.29\phi_3 + 0.321\phi_4 + 0.29\phi_5 - 0.273\phi_6 + 0.094\phi_7 - 0.094\phi_8 \\& - 0.321\phi_9 - 0.290\phi_{10} + 0.273\phi_{11} + 0.267\phi_{12} + 0.273\phi_{13} - 0.290\phi_{14} \\\psi_3 = & -0.276\phi_1 + 0.279\phi_2 + 0.291\phi_3 - 0.309\phi_4 + 0.291\phi_5 + 0.279\phi_6 - 0.057\phi_7 - \\& 0.057\phi_8 - 0.309\phi_9 + 0.291\phi_{10} + 0.279\phi_{11} - 0.276\phi_{12} + 0.279\phi_{13} + 0.291\phi_{14} \\\psi_4 = & 0.237\phi_1 + 0.248\phi_2 + 0.284\phi_3 + 0.346\phi_4 + 0.284\phi_5 + 0.248\phi_6 - 0.198\phi_7 + \\& 0.198\phi_8 + 0.346\phi_9 + 0.284\phi_{10} + 0.248\phi_{11} + 0.237\phi_{12} + 0.248\phi_{13} + 0.284\phi_{14} \\\psi_5 = & 0.327\phi_1 + 0.305\phi_2 + 0.241\phi_3 + 0.145\phi_4 + 0.241\phi_5 + 0.305\phi_6 + 0.265\phi_7 + \\& 0.265\phi_8 + 0.145\phi_9 + 0.241\phi_{10} + 0.305\phi_{11} + 0.327\phi_{12} + 0.305\phi_{13} + 0.241\phi_{14} \\\psi_6 = & 0.272\phi_1 + 0.060\phi_2 - 0.245\phi_3 + 0.168\phi_4 - 0.245\phi_5 + 0.06\phi_6 + 0.52\phi_7 - 0.52\phi_8 + \\& 0.168\phi_9 + 0.245\phi_{10} + 0.06\phi_{11} + 0.272\phi_{12} + 0.060\phi_{13} + 0.245\phi_{14} \\\psi_7 = & -0.367\phi_1 - 0.243\phi_2 + 0.045\phi_3 + 0.303\phi_4 + 0.045\phi_5 - 0.243\phi_6 + 0.388\phi_7 + \\& 0.388\phi_8 - 0.303\phi_9 + 0.045\phi_{10} + 0.243\phi_{11} + 0.367\phi_{12} + 0.243\phi_{13} + 0.045\phi_{14} \\\psi_8 = & 0.383\phi_1 + 0.164\phi_2 - 0.242\phi_3 - 0.372\phi_4 - 0.242\phi_5 + 0.164\phi_6 + 0.207\phi_7 + 0.207\phi_8 \\& - 0.354\phi_9 - 0.372\phi_{10} - 0.242\phi_{11} + 0.164\phi_{12} + 0.383\phi_{13} + 0.164\phi_{14} \\\psi_9 = & 0.405\phi_1 - 0.226\phi_2 - 0.152\phi_3 + 0.396\phi_4 - 0.152\phi_5 - 0.226\phi_6 - 0.174\phi_7 + 0.174\phi_8 \\& - 0.396\phi_9 + 0.152\phi_{10} + 0.226\phi_{11} - 0.405\phi_{12} + 0.226\phi_{13} + 0.152\phi_{14} \\\psi_{10} = & 0.409\phi_1 - 0.218\phi_2 - 0.178\phi_3 + 0.407\phi_4 - 0.178\phi_5 - 0.218\phi_6 - 0.097\phi_7 - 0.097\phi_8 \\& + 0.407\phi_9 - 0.178\phi_{10} - 0.218\phi_{11} + 0.409\phi_{12} - 0.218\phi_{13} - 0.178\phi_{14} \\\psi_{11} = & 0\phi_1 + 0.360\phi_2 + 0.360\phi_3 + 0\phi_4 - 0.360\phi_5 - 0.360\phi_6 + 0\phi_7 + 0\phi_8 + 0\phi_9 + \\& 0.005\phi_{10} + 0.005\phi_{11} + 0\phi_{12} - 0.005\phi_{13} - 0.005\phi_{14} \\\psi_{12} = & 0\phi_1 - 0.351\phi_2 - 0.351\phi_3 + 0\phi_4 + 0.351\phi_5 + 0.351\phi_6 + 0\phi_7 + 0\phi_8 + 0\phi_9 + 0.014\phi_{10} \\& + 0.014\phi_{11} + 0\phi_{12} - 0.014\phi_{13} - 0.014\phi_{14} \\\psi_{13} = & 0\phi_1 + 0.355\phi_2 + 0.355\phi_3 + 0\phi_4 + 0.355\phi_5 + 0.355\phi_6 + 0\phi_7 + 0\phi_8 - 0\phi_9 + \\& 0.005\phi_{10} - 0.005\phi_{11} - 0\phi_{12} + 0.005\phi_{13} - 0.005\phi_{14} \\\psi_{14} = & 0\phi_1 + 0.361\phi_2 + 0.361\phi_3 - 0\phi_4 + 0.361\phi_5 + 0.361\phi_6 + 0\phi_7 + 0\phi_8 + 0\phi_9 + 0.004\phi_{10} \\& - 0.004\phi_{11} + 0\phi_{12} + 0.004\phi_{13} - 0.004\phi_{14}\end{aligned}$$

### a.3. Indeks kereaktifan

#### a.3.1. Keadaan dasar

##### - Kerapatan Elektron

Kerapatan Elektron ( $q$ ) dihitung dengan menggunakan persamaan  $q_r = \sum_r n_r (c_r)^2$

$$q_1 = 2 \cdot (0.051)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.282)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.612)^2 \text{ solve, } q_1 \rightarrow 1.000478$$

$$q_2 = 2 \cdot (0.257)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.29)^2 + 2 \cdot (0.321)^2 + 2 \cdot (0.29)^2 + 2 \cdot (-0.273)^2 + 2 \cdot (0.094)^2 \text{ solve, } q_2 \rightarrow 1.000348$$

$$q_3 = 2 \cdot (-0.276)^2 + 2 \cdot (0.279)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.309)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.279)^2 + 2 \cdot (-0.057)^2 \text{ solve, } q_3 \rightarrow .9999$$

$$q_4 = 2 \cdot (0.237)^2 + 2 \cdot (0.248)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.346)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.248)^2 + 2 \cdot (-0.198)^2 \text{ solve, } q_4 \rightarrow .993818$$

$$q_5 = 2 \cdot (0.327)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.145)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.265)^2 \text{ solve, } q_5 \rightarrow 1.000782$$

$$q_6 = 2 \cdot (0.272)^2 + 2 \cdot (0.06)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.168)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.06)^2 + 2 \cdot (0.52)^2 \text{ solve, } q_6 \rightarrow .999716$$

$$q_7 = 2 \cdot (-0.367)^2 + 2 \cdot (-0.243)^2 + 2 \cdot (0.045)^2 + 2 \cdot (0.303)^2 + 2 \cdot (0.045)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.388)^2 \text{ solve, } q_7 \rightarrow .999838$$

$$q_8 = 2 \cdot (0.383)^2 + 2 \cdot (0.164)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (0.164)^2 + 2 \cdot (0.207)^2 \text{ solve, } q_8 \rightarrow .997684$$

$$q_9 = 2 \cdot (0.405)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (0.396)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.174)^2 \text{ solve, } q_9 \rightarrow .9998954$$

$$q_{10} = 2 \cdot (0.409)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (0.407)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (-0.097)^2 \text{ solve, } q_{10} \rightarrow 1.00151$$

$$q_{11} = 2 \cdot (0)^2 + 2 \cdot (0.26)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (0)^2 \text{ solve, } q_{11} \rightarrow 1.0368$$

$$q_{12} = 2 \cdot (0)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (0)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0)^2 \text{ solve, } q_{12} \rightarrow .985608$$

$$q_{13} = 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 \text{ solve, } q_{13} \rightarrow 1.00882$$

$$q_{14} = 2 \cdot (0)^2 + 2 \cdot (0.261)^2 + 2 \cdot (-0.361)^2 + 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 2 \cdot (0)^2 \text{ solve, } q_{14} \rightarrow 1.042568$$

- Orde ikatan :

Orde ikatan dhitung dengan menggunakan persamaan :  $P_{12} = \sum_j a_j c_j$

$$P_{12}=2\cdot(0.051\cdot0.068) + 2\cdot(0.267\cdot0.273) + 2\cdot(-0.276\cdot0.279) + 2\cdot(0.237\cdot0.248) + 2\cdot(0.327\cdot0.305) + 2\cdot(0.272\cdot0.06) + 2\cdot(-0.367\cdot-0.243) \rightarrow P_{12}=.526734$$

$$P_{16}=2\cdot(0.051\cdot0.068) + 2\cdot(0.267\cdot0.273) + 2\cdot(-0.276\cdot0.279) + 2\cdot(0.237\cdot0.248) + 2\cdot(0.327\cdot0.305) + 2\cdot(0.272\cdot0.06) + 2\cdot(-0.367\cdot-0.243) \rightarrow P_{16}=.526734$$

$$P_{23}=2\cdot(0.131\cdot0.068) + 2\cdot(0.29\cdot0.273) + 2\cdot(0.291\cdot0.279) + 2\cdot(0.284\cdot0.248) + 2\cdot(0.241\cdot0.305) + 2\cdot(-0.245\cdot0.06) + 2\cdot(0.045\cdot-0.243) \rightarrow P_{23}=.575138$$

$$P_{34}=2\cdot(0.131\cdot0.282) + 2\cdot(0.29\cdot0.321) + 2\cdot(0.291\cdot0.309) + 2\cdot(0.284\cdot0.346) + 2\cdot(0.241\cdot0.145) + 2\cdot(-0.245\cdot0.168) + 2\cdot(0.045\cdot0.303) \rightarrow P_{34}=.65127$$

$$P_{45}=2\cdot(0.131\cdot0.282) + 2\cdot(0.29\cdot0.321) + 2\cdot(0.291\cdot0.309) + 2\cdot(0.284\cdot0.346) + 2\cdot(0.241\cdot0.145) + 2\cdot(-0.245\cdot0.168) + 2\cdot(0.045\cdot0.303) \rightarrow P_{45}=-.65127$$

$$P_{47}=2\cdot(0.612\cdot0.282) + 2\cdot(0.094\cdot0.321) + 2\cdot(-0.057\cdot0.309) + 2\cdot(-0.198\cdot0.346) + 2\cdot(-0.265\cdot0.145) + 2\cdot(0.52\cdot0.168) + 2\cdot(0.388\cdot0.303) \rightarrow P_{47}=.566272$$

$$P_{56}=2\cdot(0.131\cdot0.068) + 2\cdot(0.29\cdot0.273) - 2\cdot(0.291\cdot0.279) + 2\cdot(0.284\cdot0.248) + 2\cdot(0.241\cdot0.305) + 2\cdot(-0.245\cdot0.06) + 2\cdot(0.045\cdot-0.243) \rightarrow P_{56}=.575138$$

$$P_{78}=2\cdot(0.612\cdot0.612) + 2\cdot(0.094\cdot-0.094) + 2\cdot(-0.057\cdot-0.057) + 2\cdot(-0.198\cdot0.198) + 2\cdot(0.265\cdot0.265) + 2\cdot(0.52\cdot-0.52) + 2\cdot(0.388\cdot-0.388) \rightarrow P_{78}=.560244$$

$$P_{89}=2\cdot(0.612\cdot0.282) + 2\cdot(-0.094\cdot0.321) + 2\cdot(-0.057\cdot0.309) + 2\cdot(0.198\cdot0.346) + 2\cdot(0.265\cdot0.145) + 2\cdot(-0.52\cdot0.168) + 2\cdot(0.388\cdot0.303) \rightarrow P_{89}=.523868$$

$$P_{910}=2\cdot(0.131\cdot0.282) + 2\cdot(-0.29\cdot0.321) + 2\cdot(0.291\cdot0.309) + 2\cdot(0.284\cdot0.346) + 2\cdot(0.241\cdot0.145) + 2\cdot(-0.245\cdot0.168) + 2\cdot(0.045\cdot0.303) \rightarrow P_{910}=-.44355$$

$$P_{914}=2\cdot(0.131\cdot0.282) + 2\cdot(-0.29\cdot0.321) + 2\cdot(0.291\cdot0.309) + 2\cdot(0.284\cdot0.346) + 2\cdot(0.241\cdot0.145) + 2\cdot(-0.245\cdot0.168) + 2\cdot(0.045\cdot0.303) \rightarrow P_{914}=-.44355$$

$$P_{1011}=2\cdot(0.131\cdot0.068) + 2\cdot(0.29\cdot0.273) + 2\cdot(0.291\cdot0.279) + 2\cdot(0.284\cdot0.248) + 2\cdot(0.241\cdot0.305) + 2\cdot(-0.245\cdot0.06) + 2\cdot(0.245\cdot0.243) \rightarrow P_{1011}=.633938$$

$$P_{1112}=2\cdot(0.051\cdot0.068) + 2\cdot(0.267\cdot0.273) + 2\cdot(-0.276\cdot0.279) + 2\cdot(0.237\cdot0.248) + 2\cdot(0.327\cdot0.305) + 2\cdot(0.272\cdot0.06) + 2\cdot(0.367\cdot0.243) \rightarrow P_{1112}=.526734$$

$$P_{1213}=2\cdot(0.051\cdot0.068) + 2\cdot(0.267\cdot0.273) + 2\cdot(-0.276\cdot0.279) + 2\cdot(0.237\cdot0.248) + 2\cdot(0.327\cdot0.305) + 2\cdot(0.272\cdot0.06) + 2\cdot(0.367\cdot0.243) \rightarrow P_{1213}=.526734$$

$$P_{1314}=2\cdot(0.131\cdot0.068) + 2\cdot(-0.29\cdot0.273) + 2\cdot(0.291\cdot0.279) + 2\cdot(0.284\cdot0.248) + 2\cdot(0.241\cdot0.305) + 2\cdot(0.245\cdot0.06) + 2\cdot(0.045\cdot0.243) \rightarrow P_{1314}=.260998$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.527 - 0.527 \text{ solve}, F_1 \rightarrow .6780508075688772935$$

$$F_2 = \sqrt{3} - 0.527 - 0.575 \text{ solve}, F_2 \rightarrow .6300508075688772935$$

$$F_3 = \sqrt{3} - 0.575 - 0.651 \text{ solve}, F_3 \rightarrow .5060508075688772935$$

$$F_4 = \sqrt{3} - 0.651 - 0.566 - 0.651 \text{ solve}, F_4 \rightarrow -.1359491924311227065$$

$$F_5 = \sqrt{3} - 0.651 - 0.575 \text{ solve}, F_5 \rightarrow .5060508075688772935$$

$$F_6 = \sqrt{3} - 0.527 - 0.575 \text{ solve}, F_6 \rightarrow .6300508075688772935$$

$$F_7 = \sqrt{3} - 0.566 - 0.560 \text{ solve}, F_7 \rightarrow .6060508075688772935$$

$$F_8 = \sqrt{3} - 0.560 - 0.524 \text{ solve}, F_8 \rightarrow .6480508075688772935$$

$$F_9 = \sqrt{3} - 0.443 - 0.443 - 0.524 \text{ solve}, F_9 \rightarrow .3220508075688772935$$

$$F_{10} = \sqrt{3} - 0.443 - 0.634 \text{ solve}, F_{10} \rightarrow .6550508075688772935$$

$$F_{11} = \sqrt{3} - 0.575 - 0.461 \text{ solve}, F_{11} \rightarrow .6960508075688772935$$

$$F_{12} = \sqrt{3} - 0.527 - 0.527 \text{ solve}, F_{12} \rightarrow .6780508075688772935$$

$$F_{13} = \sqrt{3} - 0.527 - 0.360 \text{ solve}, F_{13} \rightarrow .8450508075688772935$$

$$F_{14} = \sqrt{3} - 0.360 - 0.443 \text{ solve}, F_{14} \rightarrow .9290508075688772935$$

### 4.2.1. Keadaan tereksitasi

#### A. 1 Elektron tereksitasi ke 1 tingkat energi lebih tinggi ( orbital 1 ) -Kerapatan elektron

$$\begin{aligned} q_1 &= 2 \cdot (0.051)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.282)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.068)^2 + 1 \cdot (0.612)^2 + 1 \cdot (0.612)^2 \text{ solve, } q_1 \rightarrow 1.000478 \\ q_2 &= 2 \cdot (0.267)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.29)^2 + 2 \cdot (0.321)^2 + 2 \cdot (0.29)^2 + 2 \cdot (-0.273)^2 + 1 \cdot (0.094)^2 + 1 \cdot (-0.094)^2 \text{ solve, } q_2 \rightarrow 1.000848 \\ q_3 &= 2 \cdot (-0.276)^2 + 2 \cdot (0.279)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.309)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.279)^2 + 1 \cdot (-0.057)^2 + 1 \cdot (-0.057)^2 \text{ solve, } q_3 \rightarrow .9999 \\ q_4 &= 2 \cdot (0.237)^2 + 2 \cdot (0.248)^2 + 2 \cdot (0.281)^2 + 2 \cdot (0.346)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.248)^2 + 1 \cdot (-0.198)^2 + 1 \cdot (0.198)^2 \text{ solve, } q_4 \rightarrow .998818 \\ q_5 &= 2 \cdot (0.327)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.145)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.305)^2 + 1 \cdot (0.265)^2 + 1 \cdot (0.265)^2 \text{ solve, } q_5 \rightarrow 1.000782 \\ q_6 &= 2 \cdot (0.272)^2 + 2 \cdot (0.06)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.168)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.06)^2 + 1 \cdot (0.52)^2 + 1 \cdot (-0.52)^2 \text{ solve, } q_6 \rightarrow .999716 \\ q_7 &= 2 \cdot (-0.367)^2 + 2 \cdot (-0.243)^2 + 2 \cdot (0.045)^2 + 2 \cdot (0.303)^2 + 2 \cdot (0.045)^2 + 2 \cdot (-0.243)^2 + 1 \cdot (0.388)^2 + 1 \cdot (0.388)^2 \text{ solve, } q_7 \rightarrow .99838 \\ q_8 &= 2 \cdot (0.383)^2 + 2 \cdot (0.164)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (0.164)^2 + 1 \cdot (0.207)^2 + 1 \cdot (0.207)^2 \text{ solve, } q_8 \rightarrow .997684 \\ q_9 &= 2 \cdot (0.405)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (0.396)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (-0.226)^2 + 1 \cdot (-0.174)^2 + 1 \cdot (0.174)^2 \text{ solve, } q_9 \rightarrow .998954 \\ q_{10} &= 2 \cdot (0.409)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (0.178)^2 + 2 \cdot (0.407)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (-0.218)^2 + 1 \cdot (-0.097)^2 + 1 \cdot (-0.097)^2 \text{ solve, } q_{10} \rightarrow 1.00151 \\ q_{11} &= 2 \cdot (0)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve, } q_{11} \rightarrow 1.0368 \\ q_{12} &= 2 \cdot (0)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (0)^2 + 2 \cdot (0)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve, } q_{12} \rightarrow .985608 \\ q_{13} &= 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve, } q_{13} \rightarrow 1.0082 \\ q_{14} &= 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve, } q_{14} \rightarrow 1.042568 \end{aligned}$$

- Orde ikatan

$$\begin{aligned}
 P_{12} &= 2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (-0.367 \cdot -0.243) + 1 \cdot (0.383 \cdot 0.164) \rightarrow P_{12} = .500365 \\
 P_{16} &= 2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.257 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (-0.367 \cdot -0.243) + 1 \cdot (0.383 \cdot 0.164) \rightarrow P_{16} = .500365 \\
 P_{23} &= 2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (-0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot -0.243) + 1 \cdot (-0.242 \cdot 0.164) \rightarrow P_{23} = .546385 \\
 P_{24} &= 2 \cdot (0.131 \cdot 0.282) + 2 \cdot (0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (-0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (-0.242 \cdot -0.372) \rightarrow P_{24} = .727659 \\
 P_{45} &= 2 \cdot (0.131 \cdot 0.282) + 2 \cdot (0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (-0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (-0.242 \cdot -0.372) \rightarrow P_{45} = .727659 \\
 P_{47} &= 2 \cdot (0.612 \cdot 0.282) + 2 \cdot (0.094 \cdot 0.321) + 2 \cdot (-0.057 \cdot 0.309) + 2 \cdot (-0.198 \cdot 0.346) + 2 \cdot (-0.265 \cdot 0.145) + 2 \cdot (0.52 \cdot 0.168) + 1 \cdot (0.388 \cdot 0.303) + 1 \cdot (-0.372 \cdot 0.207) \rightarrow P_{47} = .371704 \\
 P_{56} &= 2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (-0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot -0.243) + 1 \cdot (-0.242 \cdot 0.164) \rightarrow P_{56} = .546385 \\
 P_{78} &= 2 \cdot (0.612 \cdot 0.612) + 2 \cdot (0.094 \cdot -0.094) + 2 \cdot (-0.057 \cdot -0.057) + 2 \cdot (-0.198 \cdot 0.198) + 2 \cdot (0.265 \cdot 0.265) + 2 \cdot (0.52 \cdot -0.52) + 1 \cdot (0.388 \cdot 0.388) + 1 \cdot (0.207 \cdot 0.207) \rightarrow P_{78} = .452549 \\
 P_{89} &= 2 \cdot (0.131 \cdot 0.282) + 2 \cdot (-0.094 \cdot 0.321) + 2 \cdot (-0.057 \cdot -0.309) + 2 \cdot (0.198 \cdot 0.346) + 2 \cdot (0.265 \cdot 0.145) + 2 \cdot (-0.52 \cdot 0.168) + 1 \cdot (0.388 \cdot 0.303) + 1 \cdot (0.207 \cdot -0.372) \rightarrow P_{89} = .3293 \\
 P_{910} &= 2 \cdot (0.131 \cdot 0.282) + 2 \cdot (-0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (-0.372 \cdot -0.242) \rightarrow P_{910} = .519939 \\
 P_{914} &= 2 \cdot (0.131 \cdot 0.282) + 2 \cdot (-0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (-0.372 \cdot -0.242) \rightarrow P_{914} = .519939 \\
 P_{1011} &= 2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot -0.243) + 1 \cdot (-0.242 \cdot 0.164) \rightarrow P_{1011} = .605185 \\
 P_{1112} &= 2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (0.164 \cdot 0.383) + 1 \cdot (0.164 \cdot -0.383) \rightarrow P_{1112} = .500365 \\
 P_{1213} &= 2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (0.367 \cdot -0.243) + 1 \cdot (0.383 \cdot 0.164) \rightarrow P_{1213} = .500365 \\
 P_{1314} &= 2 \cdot (0.131 \cdot 0.068) + 2 \cdot (-0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot 0.243) + 1 \cdot (0.164 \cdot -0.242) \rightarrow P_{1314} = .389751
 \end{aligned}$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.346 - 0.346 \text{ solve}, F_1 \rightarrow 1.0400508075688772935$$

$$F_2 = \sqrt{3} - 0.346 - 0.620 \text{ solve}, F_2 \rightarrow .7660508075688772935$$

$$F_3 = \sqrt{3} - 0.620 - 0.577 \text{ solve}, F_3 \rightarrow .5350508075688772935$$

$$F_4 = \sqrt{3} - 0.577 - 0.380 - 0.577 \text{ solve}, F_4 \rightarrow .1980508075688772935$$

$$F_5 = \sqrt{3} - 0.577 - 0.620 \text{ solve}, F_5 \rightarrow .5350508075688772935$$

$$F_6 = \sqrt{3} - 0.620 - 0.346 \text{ solve}, F_6 \rightarrow .7660508075688772935$$

$$F_7 = \sqrt{3} - 0.380 - 0.379 \text{ solve}, F_7 \rightarrow .9730508075688772935$$

$$F_8 = \sqrt{3} - 0.379 - 0.337 \text{ solve}, F_8 \rightarrow 1.0160508075688772935$$

$$F_9 = \sqrt{3} - 0.337 - 0.370 - 0.370 \text{ solve}, F_9 \rightarrow .6550508075688772935$$

$$F_{10} = \sqrt{3} - 0.370 - 0.679 \text{ solve}, F_{10} \rightarrow .6830508075688772935$$

$$F_{11} = \sqrt{3} - 0.679 - 0.346 \text{ solve}, F_{11} \rightarrow .7070508075688772935$$

$$F_{12} = \sqrt{3} - 0.346 - 0.346 \text{ solve}, F_{12} \rightarrow 1.0400508075688772935$$

$$F_{13} = \sqrt{3} - 0.346 - 0.384 \text{ solve}, F_{13} \rightarrow 1.0020508075688772935$$

$$F_{14} = \sqrt{3} - 0.384 - 0.370 \text{ solve}, F_{14} \rightarrow .9780508075688772935$$

## B. 1 Elektron tereksitasi ke 1 tingkat energi lebih tinggi ( orbital 2 )

### -Kerapatan elektron

$$\begin{aligned} q_1 &= 2 \cdot (0.051)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.282)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.068)^2 + 1 \cdot (0.612)^2 + 1 \cdot (0.282)^2 \text{ solve}, q_1 \rightarrow .705458 \\ q_2 &= 2 \cdot (0.267)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.29)^2 + 2 \cdot (0.321)^2 + 2 \cdot (0.29)^2 + 2 \cdot (-0.273)^2 + 1 \cdot (0.094)^2 + 1 \cdot (0.321)^2 \text{ solve}, q_2 \rightarrow 1.095053 \\ q_3 &= 2 \cdot (-0.276)^2 + 2 \cdot (0.279)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.291)^2 + 2 \cdot (-0.057)^2 + 1 \cdot (0.309)^2 \text{ solve}, q_3 \rightarrow 1.092132 \\ q_4 &= 2 \cdot (0.237)^2 + 2 \cdot (0.248)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.346)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.248)^2 + 1 \cdot (-0.198)^2 + 1 \cdot (0.346)^2 \text{ solve}, q_4 \rightarrow 1.07933 \\ q_5 &= 2 \cdot (0.327)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.145)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.305)^2 + 1 \cdot (0.265)^2 + 1 \cdot (0.145)^2 \text{ solve}, q_5 \rightarrow .951582 \\ q_6 &= 2 \cdot (0.272)^2 + 2 \cdot (0.06)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.168)^2 + 2 \cdot (0.168)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.06)^2 + 1 \cdot (0.52)^2 + 1 \cdot (0.168)^2 \text{ solve}, q_6 \rightarrow .75754 \\ q_7 &= 2 \cdot (-0.367)^2 + 2 \cdot (-0.243)^2 + 2 \cdot (0.045)^2 + 2 \cdot (0.203)^2 + 2 \cdot (0.045)^2 + 2 \cdot (-0.243)^2 + 1 \cdot (0.388)^2 + 1 \cdot (0.303)^2 \text{ solve}, q_7 \rightarrow .939645 \\ q_8 &= 2 \cdot (0.383)^2 + 2 \cdot (0.164)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (0.164)^2 + 2 \cdot (0.207)^2 + 1 \cdot (-0.372)^2 \text{ solve}, q_8 \rightarrow 1.093219 \\ q_9 &= 2 \cdot (0.405)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (0.396)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (-0.226)^2 + 1 \cdot (-0.226)^2 + 1 \cdot (-0.174)^2 + 1 \cdot (-0.396)^2 \text{ solve}, q_9 \rightarrow 1.125494 \\ q_{10} &= 2 \cdot (0.409)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (0.407)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (-0.218)^2 + 1 \cdot (-0.097)^2 + 1 \cdot (0.407)^2 \text{ solve}, q_{10} \rightarrow 1.15775 \\ q_{11} &= 2 \cdot (0)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.26)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve}, q_{11} \rightarrow 1.0368 \\ q_{12} &= 2 \cdot (0)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (0)^2 + 2 \cdot (0)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve}, q_{12} \rightarrow .982608 \\ q_{13} &= 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve}, q_{13} \rightarrow 1.0082 \\ q_{14} &= 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 1 \cdot (0)^2 + 1 \cdot (0)^2 \text{ solve}, q_{14} \rightarrow 1.042568 \end{aligned}$$



- Harga valensi bebas

$$F_r = N_{\max} - N_r$$

$$F_1 = \sqrt{3} - 0.500 - 0.500 \text{ solve, } F_1 \rightarrow .7320508075688772935$$

$$F_2 = \sqrt{3} - 0.500 - 0.546 \text{ solve, } F_2 \rightarrow .6860508075688772935$$

$$F_3 = \sqrt{3} - 0.546 - 0.728 \text{ solve, } F_3 \rightarrow .4580508075688772935$$

$$F_4 = \sqrt{3} - 0.728 - 0.728 - 0.378 \text{ solve, } F_4 \rightarrow -.1019491924311227065$$

$$F_5 = \sqrt{3} - 0.728 - 0.546 \text{ solve, } F_5 \rightarrow .4580508075688772935$$

$$F_6 = \sqrt{3} - 0.546 - 0.500 \text{ solve, } F_6 \rightarrow .6860508075688772935$$

$$F_7 = \sqrt{3} - 0.452 - 0.378 \text{ solve, } F_7 \rightarrow .9020508075688772935$$

$$F_8 = \sqrt{3} - 0.452 - 0.329 \text{ solve, } F_8 \rightarrow .9510508075688772935$$

$$F_9 = \sqrt{3} - 0.329 - 0.520 - 0.520 \text{ solve, } F_9 \rightarrow .3630508075688772935$$

$$F_{10} = \sqrt{3} - 0.520 - 0.605 \text{ solve, } F_{10} \rightarrow .6070508075688772935$$

$$F_{11} = \sqrt{3} - 0.605 - 0.500 \text{ solve, } F_{11} \rightarrow .6270508075688772935$$

$$F_{12} = \sqrt{3} - 0.500 - 0.500 \text{ solve, } F_{12} \rightarrow .7320508075688772935$$

$$F_{13} = \sqrt{3} - 0.500 - 0.389 \text{ solve, } F_{13} \rightarrow .8430508075688772935$$

$$F_{14} = \sqrt{3} - 0.520 - 0.389 \text{ solve, } F_{14} \rightarrow .8230508075688772935$$

C. 1 Elektron tereksitasi ke 2 tingkat energi lebih tinggi { orbital 1 }

- Kerapatan elektron

$$\begin{aligned}q_1 &= 2 \cdot (0.051)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.282)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.068)^2 + 1 \cdot (0.612)^2 + 1 \cdot (0.121)^2 \text{ solve, } q_1 \rightarrow .643095 \\q_2 &= 2 \cdot (0.267)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.29)^2 + 2 \cdot (0.321)^2 + 2 \cdot (0.29)^2 + 2 \cdot (-0.273)^2 + 1 \cdot (0.094)^2 + 1 \cdot (-0.29)^2 \text{ solve, } q_2 \rightarrow 1.076112 \\q_3 &= 2 \cdot (-0.276)^2 + 2 \cdot (0.279)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.309)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.279)^2 + 1 \cdot (-0.057)^2 + 1 \cdot (0.291)^2 \text{ solve, } q_3 \rightarrow 1.081332 \\q_4 &= 2 \cdot (0.237)^2 + 2 \cdot (0.248)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.346)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.248)^2 + 1 \cdot (-0.198)^2 + 1 \cdot (0.284)^2 \text{ solve, } q_4 \rightarrow 1.04027 \\q_5 &= 2 \cdot (0.327)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.145)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.305)^2 + 1 \cdot (0.255)^2 + 1 \cdot (0.241)^2 \text{ solve, } q_5 \rightarrow .988638 \\q_6 &= 2 \cdot (0.272)^2 + 2 \cdot (0.06)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.168)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.06)^2 + 1 \cdot (0.52)^2 + 1 \cdot (0.245)^2 \text{ solve, } q_6 \rightarrow .789341 \\q_7 &= 2 \cdot (-0.367)^2 + 2 \cdot (-0.243)^2 + 2 \cdot (0.045)^2 + 2 \cdot (0.303)^2 + 2 \cdot (0.045)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (-0.388)^2 + 1 \cdot (0.045)^2 \text{ solve, } q_7 \rightarrow .849861 \\q_8 &= 2 \cdot (0.383)^2 + 2 \cdot (0.164)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (0.164)^2 + 2 \cdot (0.267)^2 + 1 \cdot (-0.242)^2 \text{ solve, } q_8 \rightarrow 1.013399 \\q_9 &= 2 \cdot (0.405)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (0.396)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (-0.226)^2 + 1 \cdot (-0.174)^2 + 1 \cdot (0.152)^2 \text{ solve, } q_9 \rightarrow .991782 \\q_{10} &= 2 \cdot (0.409)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (0.407)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (-0.218)^2 + 1 \cdot (-0.097)^2 + 1 \cdot (-0.178)^2 \text{ solve, } q_{10} \rightarrow 1.022785 \\q_{11} &= 2 \cdot (0)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 1 \cdot (0)^2 + 1 \cdot (0.005)^2 \text{ solve, } q_{11} \rightarrow 1.036825 \\q_{12} &= 2 \cdot (0)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (0)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 1 \cdot (0)^2 + 1 \cdot (0.014)^2 \text{ solve, } q_{12} \rightarrow .985804 \\q_{13} &= 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 1 \cdot (0)^2 + 1 \cdot (0.005)^2 \text{ solve, } q_{13} \rightarrow 1.008225 \\q_{14} &= 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 1 \cdot (0)^2 + 1 \cdot (0.004)^2 \text{ solve, } q_{14} \rightarrow 1.042584\end{aligned}$$



- Harga valensi bebas

$$F_r = N_{\max} - N_r$$

$$F_1 = \sqrt{3} - 0.348 - 0.348 \text{ solve, } F_1 \rightarrow 1.0360508075688772935$$

$$F_2 = \sqrt{3} - 0.348 - 0.625 \text{ solve, } F_2 \rightarrow .7590508075688772935$$

$$F_3 = \sqrt{3} - 0.625 - 0.565 \text{ solve, } F_3 \rightarrow .5420508075688772935$$

$$F_4 = \sqrt{3} - 0.565 - 0.380 - 0.565 \text{ solve, } F_4 \rightarrow .2220508075688772935$$

$$F_5 = \sqrt{3} - 0.565 - 0.625 \text{ solve, } F_5 \rightarrow .5420508075688772935$$

$$F_6 = \sqrt{3} - 0.625 - 0.348 \text{ solve, } F_6 \rightarrow .7590508075688772935$$

$$F_7 = \sqrt{3} - 0.400 - 0.408 \text{ solve, } F_7 \rightarrow .9240508075688772935$$

$$F_8 = \sqrt{3} - 0.400 - 0.367 \text{ solve, } F_8 \rightarrow .9650508075688772935$$

$$F_9 = \sqrt{3} - 0.367 - 0.357 - 0.357 \text{ solve, } F_9 \rightarrow .6510508075688772935$$

$$F_{10} = \sqrt{3} - 0.357 - 0.684 \text{ solve, } F_{10} \rightarrow .6910508075688772935$$

$$F_{11} = \sqrt{3} - 0.684 - 0.348 \text{ solve, } F_{11} \rightarrow .7000508075688772935$$

$$F_{12} = \sqrt{3} - 0.348 - 0.348 \text{ solve, } F_{12} \rightarrow 1.0360508075688772935$$

$$F_{13} = \sqrt{3} - 0.348 - 0.389 \text{ solve, } F_{13} \rightarrow .9950508075688772935$$

$$F_{14} = \sqrt{3} - 0.389 - 0.357 \text{ solve, } F_{14} \rightarrow .9860508075688772935$$



D. 1 Elektron tereksitasi ke 2 tingkat energi lebih tinggi ( orbital 2 )  
 -Kerapatan elektron

$$\begin{aligned}
 q_1 &= 2 \cdot (0.051)^2 + 2 \cdot (0.068)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.282)^2 + 2 \cdot (0.131)^2 + 2 \cdot (0.068)^2 + 1 \cdot (0.612)^2 + 1 \cdot (0.068)^2 \text{ solve, } q_1 \rightarrow .695558 \\
 q_2 &= 2 \cdot (0.267)^2 + 2 \cdot (0.273)^2 + 2 \cdot (0.29)^2 + 2 \cdot (0.321)^2 + 2 \cdot (0.29)^2 + 2 \cdot (-0.273)^2 + 1 \cdot (0.094)^2 + 1 \cdot (0.273)^2 \text{ solve, } q_2 \rightarrow 1.066541 \\
 q_3 &= 2 \cdot (-0.276)^2 + 2 \cdot (0.279)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.309)^2 + 2 \cdot (0.291)^2 + 2 \cdot (0.279)^2 + 1 \cdot (-0.057)^2 + 1 \cdot (0.279)^2 \text{ solve, } q_3 \rightarrow 1.074492 \\
 q_4 &= 2 \cdot (0.237)^2 + 2 \cdot (0.248)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.346)^2 + 2 \cdot (0.284)^2 + 2 \cdot (0.248)^2 + 1 \cdot (-0.198)^2 + 1 \cdot (0.248)^2 \text{ solve, } q_4 \rightarrow 1.021118 \\
 q_5 &= 2 \cdot (0.327)^2 + 2 \cdot (0.305)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.145)^2 + 2 \cdot (0.241)^2 + 2 \cdot (0.305)^2 + 1 \cdot (0.265)^2 + 1 \cdot (0.305)^2 \text{ solve, } q_5 \rightarrow 1.023582 \\
 q_6 &= 2 \cdot (0.272)^2 + 2 \cdot (0.06)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.168)^2 + 2 \cdot (-0.245)^2 + 2 \cdot (0.06)^2 + 1 \cdot (0.52)^2 + 1 \cdot (0.06)^2 \text{ solve, } q_6 \rightarrow .732916 \\
 q_7 &= 2 \cdot (-0.367)^2 + 2 \cdot (-0.243)^2 + 2 \cdot (0.045)^2 + 2 \cdot (0.303)^2 + 2 \cdot (0.045)^2 + 2 \cdot (-0.243)^2 + 1 \cdot (0.388)^2 + 1 \cdot (0.243)^2 \text{ solve, } q_7 \rightarrow .906885 \\
 q_8 &= 2 \cdot (0.383)^2 + 2 \cdot (0.164)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (-0.372)^2 + 2 \cdot (-0.242)^2 + 2 \cdot (0.164)^2 + 1 \cdot (0.207)^2 + 1 \cdot (0.164)^2 \text{ solve, } q_8 \rightarrow .981731 \\
 q_9 &= 2 \cdot (0.405)^2 + 2 \cdot (-0.226)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (0.395)^2 + 2 \cdot (-0.152)^2 + 2 \cdot (-0.226)^2 + 1 \cdot (-0.174)^2 + 1 \cdot (0.226)^2 \text{ solve, } q_9 \rightarrow 1.019754 \\
 q_{10} &= 2 \cdot (0.409)^2 + 2 \cdot (-0.218)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (0.407)^2 + 2 \cdot (-0.178)^2 + 2 \cdot (-0.218)^2 + 1 \cdot (-0.097)^2 + 1 \cdot (-0.218)^2 \text{ solve, } q_{10} \rightarrow 1.039625 \\
 q_{11} &= 2 \cdot (0)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0.36)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.36)^2 + 2 \cdot (-0.36)^2 + 1 \cdot (0)^2 + 1 \cdot (0.005)^2 \text{ solve, } q_{11} \rightarrow 1.036825 \\
 q_{12} &= 2 \cdot (0)^2 + 2 \cdot (-0.351)^2 + 2 \cdot (0)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 2 \cdot (0.351)^2 + 1 \cdot (0)^2 + 1 \cdot (0.014)^2 \text{ solve, } q_{12} \rightarrow 985804 \\
 q_{13} &= 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 2 \cdot (0)^2 + 2 \cdot (-0.355)^2 + 2 \cdot (0.355)^2 + 1 \cdot (0)^2 + 1 \cdot (0.005)^2 \text{ solve, } q_{13} \rightarrow 1.008225 \\
 q_{14} &= 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 2 \cdot (0)^2 + 2 \cdot (0.361)^2 + 2 \cdot (-0.361)^2 + 1 \cdot (0)^2 + 1 \cdot (0.004)^2 \text{ solve, } q_{14} \rightarrow 1.042584
 \end{aligned}$$

- Orde ikatan

$$P_{12}=2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.216 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.303) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (-0.367 \cdot -0.243) + 1 \cdot (0.048 \cdot 0.36) \rightarrow P_{12}=454833$$

$$P_{16}=2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.216 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (-0.367 \cdot -0.243) + 1 \cdot (0.048 \cdot 0.36) \rightarrow P_{16}=454833$$

$$P_{25}=2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (-0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot 0.243) + 1 \cdot (0.36 \cdot 0.36) \rightarrow P_{25}=715673$$

$$P_{34}=2 \cdot (0.131 \cdot 0.282) + 2 \cdot (0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (-0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (0.36 \cdot 0) \rightarrow P_{34}=637635$$

$$P_{45}=2 \cdot (0.131 \cdot 0.282) + 2 \cdot (0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (-0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (0 \cdot -0.346) \rightarrow P_{45}=637635$$

$$P_{47}=2 \cdot (0.612 \cdot 0.282) + 2 \cdot (0.29 \cdot 0.321) + 2 \cdot (0.057 \cdot 0.309) + 2 \cdot (-0.198 \cdot 0.346) + 2 \cdot (-0.265 \cdot 0.145) + 2 \cdot (0.52 \cdot 0.168) + 1 \cdot (0 \cdot 0) \rightarrow P_{47}=-448708$$

$$P_{55}=2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (-0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot -0.243) + 1 \cdot (-0.36 \cdot -0.36) \rightarrow P_{55}=715673$$

$$P_{78}=2 \cdot (0.612 \cdot 0.612) + 2 \cdot (0.094 \cdot -0.094) + 2 \cdot (-0.057 \cdot -0.057) + 2 \cdot (-0.198 \cdot 0.198) + 2 \cdot (0.265 \cdot 0.265) + 2 \cdot (0.52 \cdot -0.52) + 1 \cdot (0.388 \cdot 0.388) + 1 \cdot (0 \cdot 0) \rightarrow P_{78}=-45997$$

$$P_{89}=2 \cdot (0.612 \cdot 0.282) + 2 \cdot (-0.094 \cdot 0.321) + 2 \cdot (-0.057 \cdot 0.309) + 2 \cdot (0.198 \cdot 0.346) + 2 \cdot (0.265 \cdot 0.145) + 2 \cdot (-0.52 \cdot 0.168) + 1 \cdot (0.388 \cdot 0.303) + 1 \cdot 0 \cdot 0 \rightarrow P_{89}=-406304$$

$$P_{910}=2 \cdot (0.131 \cdot 0.282) + 2 \cdot (-0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (0 \cdot 0.005) \rightarrow P_{910}=429915$$

$$P_{914}=2 \cdot (0.131 \cdot 0.282) + 2 \cdot (-0.29 \cdot 0.321) + 2 \cdot (0.291 \cdot 0.309) + 2 \cdot (0.284 \cdot 0.346) + 2 \cdot (0.241 \cdot 0.145) + 2 \cdot (0.245 \cdot 0.168) + 1 \cdot (0.045 \cdot 0.303) + 1 \cdot (0 \cdot -0.005) \rightarrow P_{914}=429915$$

$$P_{1011}=2 \cdot (0.131 \cdot 0.068) + 2 \cdot (0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (0.245 \cdot 0.06) + 1 \cdot (-0.045 \cdot 0.243) + 1 \cdot (0.005 \cdot 0.005) \rightarrow P_{1011}=644898$$

$$P_{1112}=2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (0.367 \cdot 0.243) + 1 \cdot (0.005 \cdot 0) \rightarrow P_{1112}=437553$$

$$P_{1213}=2 \cdot (0.051 \cdot 0.068) + 2 \cdot (0.267 \cdot 0.273) + 2 \cdot (-0.276 \cdot 0.279) + 2 \cdot (0.237 \cdot 0.248) + 2 \cdot (0.327 \cdot 0.305) + 2 \cdot (0.272 \cdot 0.06) + 1 \cdot (0.367 \cdot 0.243) + 1 \cdot (0 \cdot -0.005) \rightarrow P_{1213}=437553$$

$$P_{1314}=2 \cdot (0.131 \cdot 0.068) + 2 \cdot (-0.29 \cdot 0.273) + 2 \cdot (0.291 \cdot 0.279) + 2 \cdot (0.284 \cdot 0.248) + 2 \cdot (0.241 \cdot 0.305) + 2 \cdot (0.245 \cdot 0.06) + 1 \cdot (0.045 \cdot 0.243) + 1 \cdot (-0.005 \cdot -0.005) \rightarrow P_{1314}=350088$$

- Harga valensi bebas

$$F_r = N_{\text{maks}} - N_r$$

$$F_1 = \sqrt{3} - 0.455 - 0.716 \text{ solve}, F_1 \rightarrow .5610508075688772935$$

$$F_2 = \sqrt{3} - 0.455 - 0.455 \text{ solve}, F_2 \rightarrow .8220508075688772935$$

$$F_3 = \sqrt{3} - 0.716 - 0.638 \text{ solve}, F_3 \rightarrow .3780508075688772935$$

$$F_4 = \sqrt{3} - 0.638 - 0.638 - 0.449 \text{ solve}, F_4 \rightarrow .0070508075688772935000$$

$$F_5 = \sqrt{3} - 0.638 - 0.716 \text{ solve}, F_5 \rightarrow .3780508075688772935$$

$$F_6 = \sqrt{3} - 0.716 - 0.455 \text{ solve}, F_6 \rightarrow .5610508075688772935$$

$$F_7 = \sqrt{3} - 0.449 - 0.410 \text{ solve}, F_7 \rightarrow .8730508075688772935$$

$$F_8 = \sqrt{3} - 0.410 - 0.406 \text{ solve}, F_8 \rightarrow .9160508075688772935$$

$$F_9 = \sqrt{3} - 0.406 - 0.430 - 0.430 \text{ solve}, F_9 \rightarrow .4660508075688772935$$

$$F_{10} = \sqrt{3} - 0.430 - 0.645 \text{ solve}, F_{10} \rightarrow .6570508075688772935$$

$$F_{11} = \sqrt{3} - 0.645 - 0.437 \text{ solve}, F_{11} \rightarrow .6500508075688772935$$

$$F_{12} = \sqrt{3} - 0.437 - 0.437 \text{ solve}, F_{12} \rightarrow .8580508075688772935$$

$$F_{13} = \sqrt{3} - 0.437 - 0.350 \text{ solve}, F_{13} \rightarrow .9450508075688772935$$

$$F_{14} = \sqrt{3} - 0.350 - 0.430 \text{ solve}, F_{14} \rightarrow .9520508075688772935$$



## LAMPIRAN C

### VARIASI $k_{CO}$ UNTUK FENOLFTALEIN DALAM SUASANA BASA

Perhitungan  $\lambda$  maksimum phenolptalein dengan memvariasikan harga  $k_C$  antara 0.1-1

$$1. k_{CO} = 1$$

$x+2 \quad 1 \quad 0 \quad 0$	$1$
$1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0$	$-1$
$0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-2.6167755365590546159$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-2.5481436997458190512$
$0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 1 \quad 0 \quad 0$	$-2.1672691644967520796$
$0 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-1.8926773878349851075$
$0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 0 \quad 0$	$-1.296068415296627794$
$0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad x \quad 1 \quad 0 \quad 0$	$-1.1217659567024037564$
$0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0$	$-0.091816878215702707497$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$	$.40060292821255357403$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$	$.85836222028846476317$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0$	$1.0425115774680271517$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0$	$1.3097870021385552137$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$1.4697122145708179172$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0$	$2.0749547281563904869$
$0 \quad 0 \quad 1 \quad x \quad 2$	$2.2953108085934655318$

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{(-.0918168782157 - .400602928212) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol}} = \frac{sec \cdot mol}{\lambda}$$

solve , $\lambda \rightarrow 771.41468008884739788$  nm

$$2. k_{cx} = 0.9$$

x+2	0.9	0	0	0	0	0	0	0	0	0	0	0	0	-3.6265906458769951894
0.9	x	1	0	0	0	1	0	0	0	0	0	0	0	-2.1705686402092637527
0	1	x	1	0	0	0	0	0	0	0	0	0	0	-2.1705686402092637527
0	0	1	x	1	0	0	0	0	0	0	0	0	0	-1.6283791127181430161
0	0	0	1	x	1	0	1	0	0	0	0	0	0	-1.2598105633758029294
0	0	0	0	1	x	1	0	0	0	0	0	0	0	-1.2598105633758029294
0	1	0	0	0	1	x	0	0	0	0	0	0	0	.66226891904713808389
0	0	0	0	1	0	0	x	1	0	0	0	0	0	-.15793840724625132514
0	0	0	0	0	0	1	x	1	0	0	1	0	0	.37087716344618915957
0	0	0	0	0	0	0	1	x	1	0	0	0	0	.66226891904713808389
0	0	0	0	0	0	0	0	1	x	1	0	0	0	1.0149808153902353822
0	0	0	0	0	0	0	0	0	1	x	1	0	0	1.0149808153902353822
0	0	0	0	0	0	0	0	0	0	1	x	1	0	1.2292924440286587586
0	0	0	0	0	0	0	0	0	0	0	1	x	1	1.6985296833538622835
0	0	0	0	0	0	0	0	0	0	0	0	1	x	1.6985296833538622835
0	0	0	0	0	0	0	0	0	0	0	0	0	0.9	2.514881053591343067
0	0	0	0	0	0	0	0	0	0	0	0	0	x+2	

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{mol \cdot sec \cdot mol}$$

$$(-.1579384072462 - .3708771634461) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{sec \cdot mol}{\lambda}$$

solve,  $\lambda \rightarrow 718.32201715972590504 \text{ nm}$

3.  $k_{cx} = 0.8$

$x+2$	0.8	0	0	0	0	0	0	0	0	0	0	0	0	- 2.7095440619784127355
0.8	$x$	1	0	0	0	1	0	0	0	0	0	0	0	- 2.7095440619784127355
0	1	$x$	1	0	0	0	0	0	0	0	0	0	0	- 2.0374218152446155269
0	0	1	$x$	1	0	0	0	0	0	0	0	0	0	- 1.5881263850127928
0	0	0	1	$x$	1	0	1	0	0	0	0	0	0	- 1.5881263850127928
0	0	0	0	1	$x$	1	0	0	0	0	0	0	0	- .99157525923492671859
0	1	0	0	0	1	$x$	0	0	0	0	0	0	0	- .99157525923492671859
0	0	0	0	1	0	0	$x$	1	0	0	0	0	0	- .13735758974458873599
0	0	0	0	0	0	1	$x$	1	0	0	1	0	0	.36003616607599650337
0	0	0	0	0	0	0	1	$x$	1	0	0	0	0	.68725207498588451071
0	0	0	0	0	0	0	0	1	$x$	1	0	0	0	.98510369565988694945
0	0	0	0	0	0	0	0	0	1	$x$	1	0	0	.98510369565988694945
0	0	0	0	0	0	0	0	0	0	1	$x$	1	0	1.313367679118754724
0	0	0	0	0	0	0	0	0	0	1	0	$x$	1	1.313367679118754724
0	0	0	0	0	0	0	0	0	0	0	1	$x$	0.8	2.2503731490640283053
0	0	0	0	0	0	0	0	0	0	0	0	0.8	$x+2$	2.2503731490640283053

$$(-.13735758974458 - .3600361660759) \cdot 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}}$$

solve  $\lambda \rightarrow 763.7005149342578917$

4.  $k_{cx} = 0.7$

$x+2$	0.7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	- 2.8296095910628396038
0.7	x	1	0	0	0	1	0	0	0	0	0	0	0	0	0	- 2.4588926225737541574
0	1	x	1	0	0	0	0	0	0	0	0	0	0	0	0	- 2.1062879884747967132
0	0	1	x	1	0	0	0	0	0	0	0	0	0	0	0	- 2.1062879884747967132
0	0	0	1	x	1	0	1	0	0	0	0	0	0	0	0	- 1.2410522037676151655
0	0	0	0	1	x	1	0	0	0	0	0	0	0	0	0	- 1.2410522037676151655
0	1	0	0	0	1	x	0	0	0	0	0	0	0	0	0	- .64373886003663443229
0	0	0	0	1	0	0	x	1	0	0	0	0	0	0	0	- .22866464442713264083
0	0	0	0	0	0	1	x	1	0	0	0	1	0	0	0	.3201299927197032887
0	0	0	0	0	0	0	1	x	1	0	0	0	0	0	0	.64373886003663443229
0	0	0	0	0	0	0	0	0	1	x	1	0	0	0	0	.9397708660145310553
0	0	0	0	0	0	0	0	0	0	1	x	1	0	0	0	.9397708660145310553
0	0	0	0	0	0	0	0	0	0	0	1	x	1	0	0	1.4265124981230506071
0	0	0	0	0	0	0	0	0	0	1	0	0	1	x	1	1.4265124981230506071
0	0	0	0	0	0	0	0	0	0	0	0	0	1	x	0.7	1.9676821950453129004
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7	x + 2	2.3837532611626376632

$$(-.22866464442713 - .3201299927197) \sim 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}} \cdot \lambda$$

$$\text{solve } \lambda \rightarrow 692.17124536811002498 \text{ nm}$$

5.  $k_{cx} = 0.6$

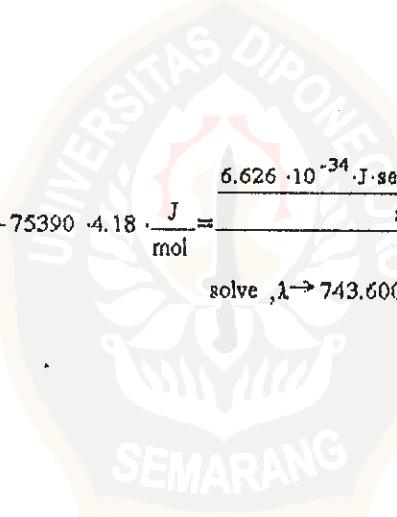
$x+2$	0.6	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	- 4.3491563311785810592
0.6	$x$	1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0	- 2.1248817649843975372
0	1	$x$ 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	- 2.1248817649843975372
0	0	1 $x$ 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0	- 1.035668170588296534
0	0	0 1 $x$ 1 0 1 0 0 0 0 0 0 0 0 0 0 0	- 1.035668170588296534
0	0	0 0 1 $x$ 1 0 0 0 0 0 0 0 0 0 0 0 0 0	.88474487665647678273
0	1	0 0 0 1 $x$ 0 0 0 0 0 0 0 0 0 0 0 0 0	.80368902368540964437
0	0	0 0 0 1 0 0 $x$ 1 0 0 0 0 0 0 0 0 0	.17151517952849052412
0	0	0 0 0 0 0 0 1 $x$ 1 0 0 0 1 0 0 0	.29751343333718623263
0	0	0 0 0 0 0 0 0 1 $x$ 1 0 0 0 0 0 0	.80368902368540964437
0	0	0 0 0 0 0 0 0 0 1 $x$ 1 0 0 0 0 0	.86766206216990406194
0	0	0 0 0 0 0 0 0 0 0 1 $x$ 1 0 0 0 0	.97186253129870761045
0	0	0 0 0 0 0 0 0 0 0 0 1 $x$ 1 0 0	.97186253129870761045
0	0	0 0 0 0 0 0 0 0 1 0 0 0 1 $x$ 1 0	1.5514200849233743316
0	0	0 0 0 0 0 0 0 0 0 0 0 0 0 1 $x$ 0.6	1.5514200849233743316
0	0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.6 $x+2$	3.1221535779285016185

$$(-.1715151795284 - .29751343333718) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{\lambda} \cdot sec \cdot mol$$

$$\text{solve, } \lambda \rightarrow 809.88634174037139775 \text{ nm}$$

$$6. k_{cx} = 0.5$$

$x+2 \quad 0.5 \quad 0 \quad 0$	$-3.5277730972103650678$
$0.5 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0$	$-2.0391513719503666171$
$0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-2.0391513719503666171$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-1.5496626542319749494$
$0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 1 \quad 0 \quad 0$	$-1.5496626542319749494$
$0 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$-95720161946452112619$
$0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 0 \quad 0$	$-95720161946452112619$
$0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$	$-23119125592824994046$
$0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0$	$.27964765818295946528$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$	$.49306146937343650106$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0 \quad 0$	$.95229705482888682295$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0 \quad 0$	$1.1281565480767951605$
$0 \quad 0 \quad 1 \quad x \quad 1 \quad 0 \quad 0$	$1.1281565480767951605$
$0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad x \quad 1$	$1.6641421087061294137$
$0 \quad 0 \quad 1 \quad x \quad 0.5$	$1.6641421087061294137$
$0 \quad 0 \quad 0.5 \quad x+2$	$2.5275150872280814582$

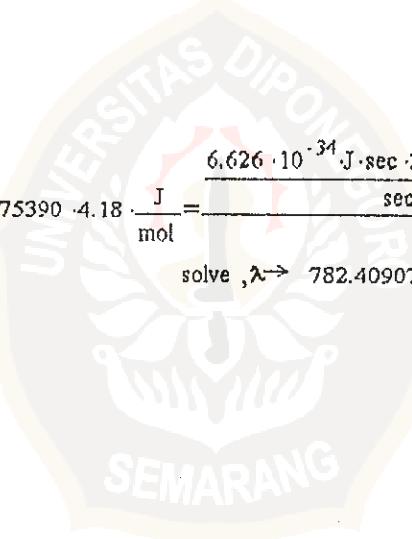


$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{mol \cdot \lambda} = \frac{sec \cdot mol}{\lambda}$$

solve,  $\lambda \rightarrow 743.60009966384462942 \cdot nm$

$$7. k_{cx} = 0.4$$

x+2 0.4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	- 2.859915006967899504
0.4 x 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0	- 2.859915006967899504
0 1 x 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0	- 1.5673088402408550639
0 0 1 x 1 0 0 0 0 0 0 0 0 0 0 0 0 0	- 1.5673088402408550639
0 0 0 1 x 1 0 1 0 0 0 0 0 0 0 0 0 0	- 1.4021806166627099209
0 0 0 0 1 x 1 0 0 0 0 0 0 0 0 0 0 0	- 1.0334572833959312488
0 1 0 0 0 1 x 0 0 0 0 0 0 0 0 0 0 0	- 1.0334572833959312488
0 0 0 0 1 0 0 x 1 0 0 0 0 0 0 0 0	- .21796252620711152049
0 0 0 0 0 0 1 x 1 0 0 0 1 0 0 0 0	.26753780640984690996
0 0 0 0 0 0 0 1 x 1 0 0 0 0 0 0 0	.7297176040270390137
0 0 0 0 0 0 0 0 1 x 1 0 0 0 0 0 0	.95545050680870398549
0 0 0 0 0 0 0 0 0 1 x 1 0 0 0 0 0	1.1285216375527669623
0 0 0 0 0 0 0 0 0 0 1 x 1 0 0 0 0	1.1285216375527669623
0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 x 1 0	1.4716160322255840275
0 0 0 0 0 0 0 0 0 0 0 0 0 1 x 0.4	2.1597876937782816204
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.4 x+2	2.1597876937782816204


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$$(-.2179625262071 - .2675378064098) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{6,626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{sec \cdot mol}$$
 solve,  $\lambda \rightarrow 782.40907765754443237 \text{ nm}$

8.  $k_{cx} = 0.3$

x+2	0.3	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0	- 2.7143551710696988537
0.3	x	1 0 0 0 1 0 0 0 0 0 0 0 0 0 0	0	- 2.3436392768192478532
0	1	x 1 0 0 0 0 0 0 0 0 0 0 0 0 0	0	- 2.3436392768192478532
0	0	1 x 1 0 0 0 0 0 0 0 0 0 0 0 0	0	- 1.5900980323851817403
0	0	0 1 x 1 0 1 0 0 0 0 0 0 0 0 0	0	- 1.5900980323851817403
0	0	0 0 1 x 1 0 0 0 0 0 0 0 0 0 0	0	.96144264854502924834
0	1	0 0 0 1 x 0 0 0 0 0 0 0 0 0 0	0	.96144264854502924834
0	0	0 0 1 0 0 x 1 0 0 0 0 0 0 0 0	0	.27567547931335619162
0	0	0 0 0 0 0 0 1 x 1 0 0 0 1 0 0	0	.2530337858741170522
0	0	0 0 0 0 0 0 0 1 x 1 0 0 0 0 0	0	.46468453422901125971
0	0	0 0 0 0 0 0 0 0 1 x 1 0 0 0 0	0	.97748743071895695369
0	0	0 0 0 0 0 0 0 0 0 1 x 1 0 0 0	0	.97748743071895695369
0	0	0 0 0 0 0 0 0 0 0 0 1 x 1 0 0	0	1.3232449201226405043
0	0	0 0 0 0 0 0 0 0 0 1 0 0 0 1 x 1	0	1.3232449201226405043
0	0	0 0 0 0 0 0 0 0 0 0 0 0 1 x 0.3	0.3	2.1952883062768360103
0	0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.3	x+2	2.1952883062768360103

solve , x →

$(-.27567547931335 \quad - .26303378587411 \quad ) \cdot 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}} \cdot \lambda$

solve ,  $\lambda \rightarrow 705.12963483758264448 \cdot \text{nm}$

9.  $k_{cx} = 0.2$

x+2	0.2	0	0	0	0	0	0	0	0	0	0	0	- 2.4511160256286596576
0.2	x	1	0	0	0	1	0	0	0	0	0	0	- 2.3052227441625858842
0	1	x	1	0	0	0	0	0	0	0	0	0	- 2.3052227441625858842
0	0	1	x	1	0	0	0	0	0	0	0	0	- 1.5049482143692262812
0	0	0	1	x	1	0	1	0	0	0	0	0	- 1.5049482143692262812
0	0	0	0	1	x	1	0	0	0	0	0	0	- 1.0587155879545501637
0	1	0	0	0	1	x	0	0	0	0	0	0	- 1.0587155879545501637
0	0	0	0	1	0	0	x	1	0	0	0	0	- .22612916454279514346
0	0	0	0	0	0	1	x	1	0	0	1	0	.26969657645634229011
0	0	0	0	0	0	0	1	x	1	0	0	0	.81359860197186127832
0	0	0	0	0	0	0	0	1	x	1	0	0	.93139303314056989638
0	0	0	0	0	0	0	0	0	1	x	1	0	1.1340455412090291608
0	0	0	0	0	0	0	0	0	0	1	x	1	0.1340455412090291608
0	0	0	0	0	0	0	0	0	0	0	1	x	1.4589746871026447466
0	0	0	0	0	0	0	0	0	0	0	0	1	2.1652307529992127414
0	0	0	0	0	0	0	0	0	0	0	0	0.2	2.1652307529992127414
													solve , x $\rightarrow$

( - .2261291645427 - .2696965764563 ) - 75390 - 4.18 
$$\frac{\text{J}}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}} \lambda$$
  
solve ,  $\lambda \rightarrow 766.11566531380690539 \text{ nm}$



**LAMPIRAN D**  
**VARIASI  $k_{CN}$  UNTUK FENOLFTALEIN DALAM SUASANA BASA**

Perhitungan  $\lambda$  maksimum metil kuning dengan memvariasikan harga kex antara 0,1-1

$$1. k_{ex} = 1$$

$z \ 1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-3.2743084524972878323$
$1 \ z \ 1 \ 0$	$-1.9165540882109887057$
$0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.9165540882109887057$
$0 \ 0 \ 1 \ z \ 1 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.2158067912388913965$
$0 \ 0 \ 0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$.027668242646176423149$
$1 \ 0 \ 0 \ 0 \ 1 \ x \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$.31898895652288986623$
$0 \ 0 \ 0 \ 1 \ 0 \ 0 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$.82563978315099568851$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1.3019456740924414996$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1.7419513819499772422$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$2.3297494780762088319$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z+1.5 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$1$

$$( -0.27668242646176423 - .31898895652288986623 + .82563978315099568851 + 1.3019456740924414996 + 1.7419513819499772422 + 2.3297494780762088319 ) \frac{6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \text{ nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}} \text{ solve } \lambda \rightleftharpoons 1095.7795434676840488 \text{ nm}$$

2.  $k_{cx} = 0.9$

$$\left[ \begin{array}{cccccc|ccccc|c} x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -2.5791753276187063476 \\ 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.5791753276187063476 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.5786166774254152555 \\ 0 & 0 & 1 & x & 1 & 0 & 0.9 & 0 & 0 & 0 & 0 & 0 & -1.293875106174309598 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -.81454088212299401146 \\ 1 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 & 0 & 0 & 0 & -.81454088212299401146 \\ 0 & 0 & 0 & 0.9 & 0 & 0 & x+1.5 & 0.9 & 0 & 0 & 0 & 0 & -.356522368011108408778 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.9 & x+1.5 & 0.9 & 0 & 0 & 0 & .21468832595418448959 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.9 & x & 1 & 0 & 0 & .21468832595418448959 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 1.1402830431619782884 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 1.1402830431619782884 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0.293875106174309598 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 2.0934089628768750519 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & x & 2.0934089628768750519 \end{array} \right] \text{ solve } ,x \rightarrow$$

$$(-.356522368011108408 - .21468832595418448) \cdot 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}}$$

$$\text{solve } ,\lambda \rightarrow 665.0083261017273467 \text{ nm}$$

3.  $K_{cx} = 0.8$

$$\left[ \begin{array}{cccccc|cccccc|c} x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 & 0.8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.8 & 0 & 0 & x+1.5 & 0.8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.8 & x+1.5 & 0.8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.8 & x & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x \end{array} \right] \xrightarrow{\text{solve }, x} \left[ \begin{array}{c} 1 \\ -3.1358391418481177997 \\ -1.8263033071274837361 \\ -1.8263033071274837361 \\ -1.1929401784901918405 \\ -.452656043031642923 \\ .09605472505491557999 \\ .09605472505491557999 \\ .84131375457045606858 \\ 1.4092432088671302462 \\ 1.5961766360212750626 \\ 2.3488413862086591953 \\ -1 \\ -1 \end{array} \right]$$

$$(-.452656043031642 - .09605472505491557) - 75390 \cdot 4.18 \cdot \frac{J}{\text{mol}} = \frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{sec} \cdot \text{mol}}$$

$$\text{solve } J \Rightarrow 692.2770420013755158 \text{ nm}$$

$$4. k_{cx} = 0.7$$

x	1	0	0	0	1	0	0	0	0	0	0	0	- 2.2341053712318578371
1	x	1	0	0	0	0	0	0	0	0	0	0	- 2.1963919982533006419
0	1	x	1	0	0	0	0	0	0	0	0	0	- 2.1963919982533006419
0	0	1	x	1	0	0.7	0	0	0	0	0	0	- 1.1879138523511852661
0	0	0	1	x	1	0	0	0	0	0	0	0	- 1.1879138523511852661
1	0	0	0	1	x	0	0	0	0	0	0	0	.83514078873266323477
0	0	0	0.7	0	0	x + 1.5	0.7	0	0	0	0	0	-.49847921020980169319
0	0	0	0	0	0	0.7	x + 1.5	0.7	0	0	0	0	.04074699141130714908
0	0	0	0	0	0	0	0.7	x + 1	0	0	0	1	.04074699141130714908
0	0	0	0	0	0	0	0	1	x + 1	0	0	0	.83514078873266323477
0	0	0	0	0	0	0	0	0	1	x + 1	0	0	1.1062050746158609955
0	0	0	0	0	0	0	0	0	0	1	x + 1	0	1.1062050746158609955
0	0	0	0	0	0	0	0	0	0	0	1	x	2.0720639413290464216
0	0	0	0	0	0	0	0	1	0	0	0	1	2.0720639413290464216

solve ,x →

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{sec \cdot mol}$$

$$(-.498479210209801 - .040746991411307) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{}{\lambda}$$

solve ,λ → 704.45365285156662516 · nm

$$5. k_{cx} = 0.6$$

x 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0	-3.2184300705146256117
1 x 1 0 0 0 0 0 0 0 0 0 0 0 0 0	-2.4260377462601377416
0 1 x 1 0 0 0 0 0 0 0 0 0 0 0 0	-2.4260377462601377416
0 0 1 x 1 0 0.6 0 0 0 0 0 0 0 0 0	-87476176199068850792
0 0 0 1 x 1 0 0 0 0 0 0 0 0 0 0 0	-87476176199068850792
1 0 0 0 1 x 0 0 0 0 0 0 0 0 0 0 0	.44891439435407404814
0 0 0 0.6 0 0 x+1.5 0.6 0 0 0 0 0 0 0	.43639241261259457392
0 0 0 0 0 0 0.6 x+1.5 0.6 0 0 0 0 0 0	.05691812217564534135
0 0 0 0 0 0 0 0.6 x 1 0 0 0 0 1	.44891439435407404814
0 0 0 0 0 0 0 0 0 1 x 1 0 0 0 0	.61374772991938404353
0 0 0 0 0 0 0 0 0 0 1 x 1 0 0	.61374772991938404353
0 0 0 0 0 0 0 0 0 0 0 1 x 1 0	1.8720511644599968704
0 0 0 0 0 0 0 0 0 0 0 0 1 x 1	1.8720511644599968704
0 0 0 0 0 0 0 0 0 1 0 0 0 1 x	2.6136712778218055395

solve ,x →

$$\frac{6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{(-.436392412612594 - .056918122175645) \cdot 75390 \cdot 4.18} \cdot \frac{J}{\text{mol}} = \frac{\text{sec} \cdot \text{mol}}{\lambda}$$

solve ,λ → 770.02180301769830233 nm

$$6. k_{ex} = 0.5$$

x 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0	1
1 x 1 0 0 0 0 0 0 0 0 0 0 0 0 0	- 2.5995508132694575386
0 1 x 1 0 0 0 0 0 0 0 0 0 0 0 0	- 2.5995508132694575386
0 0 1 x 1 0 0.5 0 0 0 0 0 0 0 0 0	- 1.3104949377979264262
0 0 0 1 x 1 0 0 0 0 0 0 0 0 0 0 0	- 1.3104949377979264262
1 0 0 0 1 x 0 0 0 0 0 0 0 0 0 0 0	.91311177457075338782
0 0 0 0.5 0 0 x+ 1.5 0.5 0 0 0 0 0 0 0	.91311177457075338782
0 0 0 0 0 0 0.5 x+ 1.5 0.5 0 0 0 0 0 0 0	.70739991265511000351
0 0 0 0 0 0 0 0.5 x 1 0 0 0 1 0 0	0.7131289421195205937
0 0 0 0 0 0 0 0 1 x 1 0 0 0 0 0	0.7131289421195205937
0 0 0 0 0 0 0 0 0 1 x 1 0 0 0 0	.70739991265511000351
0 0 0 0 0 0 0 0 0 0 1 x 1 0	1.0926230549414587631
0 0 0 0 0 0 0 0 0 0 0 1 x 1	2.0129330166105659152
0 0 0 0 0 0 0 0 0 1 0 0 0 1 x	2.0129330166105659152

$$\left( - .70739991265511000 - 0.7131289421195205 \right) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{\lambda}$$

solve , $\lambda \rightarrow 267.40735759678103634$  nm

7.  $k_{cx} = 0.4$

$$\left| \begin{array}{ccccccccc|ccccc} x & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.4 & 0 & 0 & x+1.5 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.4 & x+1.5 & 0.4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.4 & x & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x \end{array} \right| \xrightarrow{\text{solve , } x} \left| \begin{array}{cccccc} 1 \\ -1 \\ -2.2320209548153111477 \\ 2.2320209548153111477 \\ -1.5017627742325157935 \\ -1.5017627742325157935 \\ -.94865358806959159446 \\ -.67205926414834763 \\ .08985313267500849146 \\ .94865358806959159446 \\ 1.0507501671716076302 \\ 1.0507501671716076302 \\ 2.0184511128915101862 \\ 2.0184511128915101862 \end{array} \right|$$

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{(-.672059264148347) - .089853132675008491) \cdot 75390 \cdot 4.18 \cdot \frac{J}{mol}} = \frac{sec \cdot mol}{\lambda}$$

solve ,  $\lambda \rightarrow 498.56108002575687662 \text{ nm}$

$$8. k_{cx} = 0.3$$

$x \ 1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-2.592629271974972665$
$1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.8476246558527231868$
$0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.8476246558527231868$
$0 \ 0 \ 1 \ x \ 1 \ 0 \ 0.3 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.1583579795965358936$
$0 \ 0 \ 0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.084443382718499009$
$1 \ 0 \ 0 \ 0 \ 1 \ x \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.084443382718499009$
$0 \ 0 \ 0 \ 0.3 \ 0 \ 0 \ x+1.5 \ 0.3 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$.70820778981617723952$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0.3 \ x+1.5 \ 0.3 \ 0 \ 0 \ 0 \ 0 \ 0$	$.08868941957188503239$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0.3 \ x \ 1 \ 0 \ 0 \ 0 \ 1$	$.08868941957188503239$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x \ 1 \ 0 \ 0 \ 0$	$.70820778981617723952$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x \ 1 \ 0$	$1.1006291664601595262$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x \ 1$	$1.1006291664601595262$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x$	$2.0282460919941438644$
	$2.0282460919941438644$

solve ,x →

$$\frac{6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{(-.708207789816177) - .088689419571885} \approx 75390 \cdot 4.18 \cdot \frac{\text{J}}{\text{mol}} = \frac{\text{sec} \cdot \text{mol}}{\lambda}$$

solve , $\lambda \rightarrow 476.67360729868792673 \text{ nm}$

$$9. K_{CX} = 0.2$$

x 1 0 0 0 1 0 0	- 2.776334044406892852
1 x 1 0 0 0 0 0	- 1.9209384999761107931
0 1 x 1 0 0 0 0	- 1.9209384999761107931
0 0 1 x 1 0 0.2 0	- 1.4290372708056707031
0 0 0 1 x 1 0 0	- 1.4290372708056707031
1 0 0 0 1 x 0 0	- .54989281067867190185
0 0 0 0.2 0 0 x+1.5 0.2	- .41800433806700227353
0 0 0 0 0 0 0.2 x+1.5 0.2	.54989281067867190185
0 0 0 0 0 0 0.2 x 1 0 0 0 1	.59238763264105835413
0 0 0 0 0 0 0 1 x 1 0 0 0	.59238763264105835413
0 0 0 0 0 0 0 0 1 x 1 0 0	1.3278588205592213972
0 0 0 0 0 0 0 0 0 1 x 1 0	1.3278588205592213972
0 0 0 0 0 0 0 0 0 0 1 x 1	2.0767913194971212094
0 0 0 0 0 0 0 0 0 1 x	2.0767913194971212094

solve ,x →

$$\frac{6.626 \cdot 10^{-34} \cdot J \cdot sec \cdot 3 \cdot 10^{17} \cdot nm \cdot 6.022 \cdot 10^{23}}{mol}$$

$$(-.4180043380670022 - .5498928106786719) \cdot -75390 \cdot 4.18 \cdot \frac{J}{mol} = \frac{sec \cdot mol}{\lambda}$$

solve ,λ → 392.4589177037424238 · nm

$$10. k_{cx} = 0.1$$

$x \ 1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-2.836559665955157145$
$1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.7338804769326233196$
$0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.7338804769326233196$
$0 \ 0 \ 1 \ x \ 1 \ 0 \ 0.1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.1328361797527406776$
$0 \ 0 \ 0 \ 1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-1.1328361797527406776$
$1 \ 0 \ 0 \ 0 \ 1 \ x \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$.83299034459011684788$
$0 \ 0 \ 0 \ 0.1 \ 0 \ 0 \ x+1.5 \ 0.1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$	$-.80725143067566131414$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0.1 \ x+1.5 \ 0.1 \ 0 \ 0 \ 0 \ 0 \ 0$	$.08659610487252237073$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0.1 \ x \ 1 \ 0 \ 0 \ 0 \ 0 \ 1$	$.80725143067566131414$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x \ 1 \ 0 \ 0 \ 0$	$.94486846711263093654$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z \ 1 \ 0 \ 0$	$.94486846711263093654$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x \ 1 \ 0$	$1.4119611693293415249$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ z \ 1$	$1.577527430623005915$
$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ x$	$2.2722996023644915953$

$$\text{solve ,x } \rightarrow$$

$$\frac{6.626 \cdot 10^{-34} \cdot \text{J} \cdot \text{sec} \cdot 3 \cdot 10^{17} \cdot \text{nm} \cdot 6.022 \cdot 10^{23}}{\text{mol}} = \frac{\text{sec} \cdot \text{mol}}{\lambda}$$

$$\text{solve ,} \lambda \rightarrow 424.9716560579908657 \text{ nm}$$

