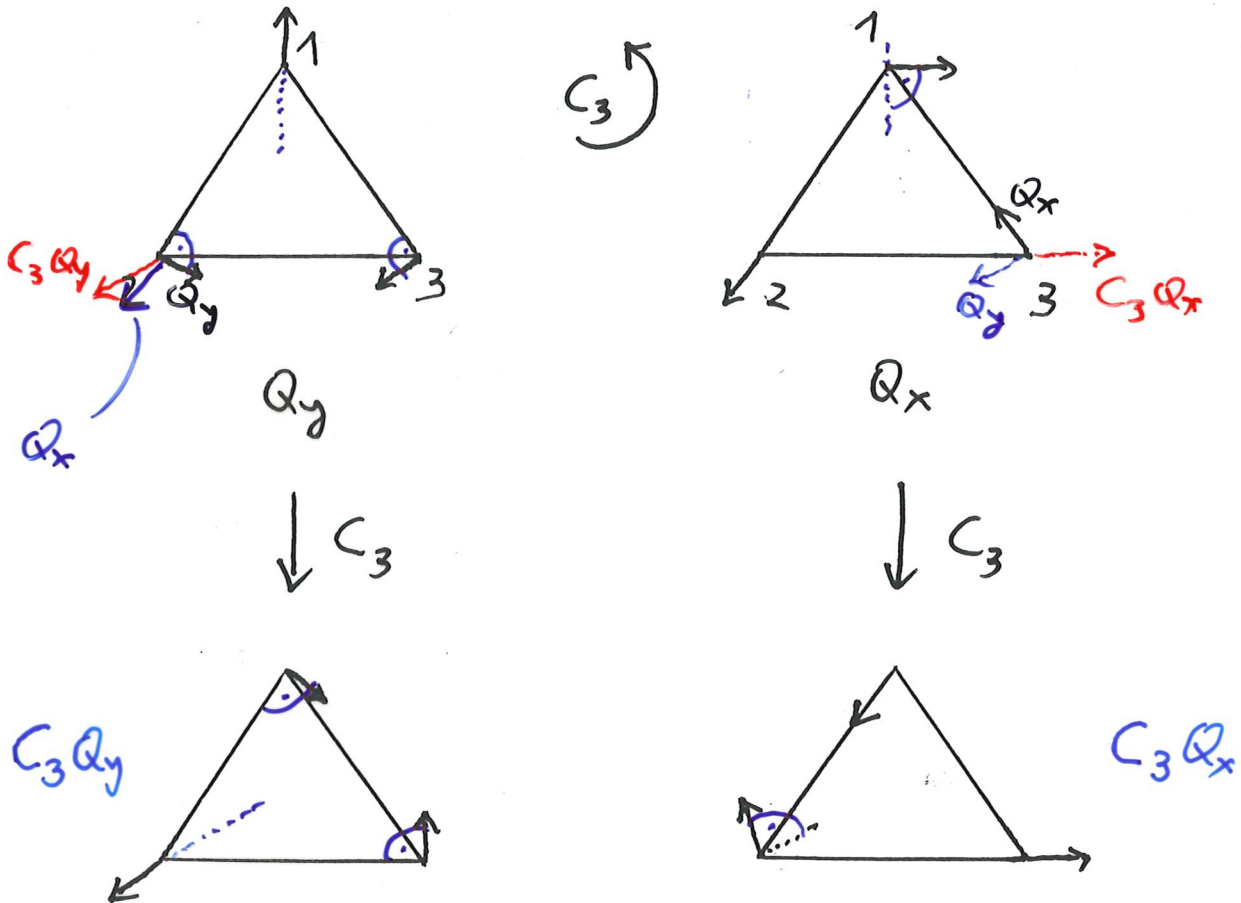


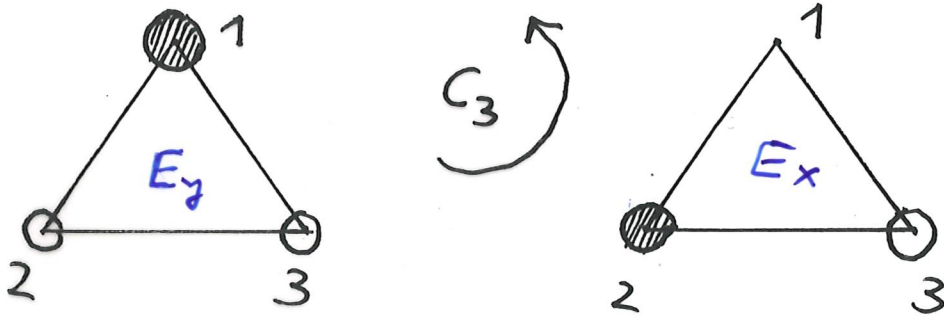
Symmetriegerichte Kernkoord. des Dreizentren-P.



$$\begin{cases} C_3 Q_y = \frac{1}{2} \sqrt{3} Q_x - \frac{1}{2} Q_y \\ C_3 Q_x = -\frac{1}{2} \sqrt{3} Q_y - \frac{1}{2} Q_x \end{cases}$$

(geometrische Überlegungen)

Symmetriegerichte u. WF des Dreizentren-Problems



$$\begin{cases} |E_y\rangle = \frac{1}{\sqrt{6}} (2|1\rangle - |2\rangle - |3\rangle) \\ |E_x\rangle = \frac{1}{\sqrt{2}} (|2\rangle - |3\rangle) \end{cases}$$

$$\Rightarrow \begin{cases} C_3 |E_y\rangle = \frac{1}{\sqrt{6}} (2|2\rangle - |3\rangle - |1\rangle) \\ C_3 |E_x\rangle = \frac{1}{\sqrt{2}} (|3\rangle - |1\rangle) \end{cases}$$

$$\begin{aligned} \Rightarrow & \underbrace{-\frac{1}{2} |E_x\rangle} - \underbrace{\frac{\sqrt{3}}{2} |E_y\rangle} = \\ & = -\frac{1}{2\sqrt{2}} |2\rangle + \frac{1}{2\sqrt{2}} |3\rangle - \frac{1}{\sqrt{2}} |1\rangle + \frac{1}{2\sqrt{2}} |2\rangle + \frac{1}{2\sqrt{2}} |3\rangle \\ & = \frac{1}{\sqrt{2}} |3\rangle - \frac{1}{\sqrt{2}} |1\rangle = C_3 |E_x\rangle \end{aligned}$$

und analog für $C_3 |E_y\rangle$:

$$-\frac{1}{2} |E_y\rangle + \frac{\sqrt{3}}{2} |E_x\rangle = C_3 |E_y\rangle$$