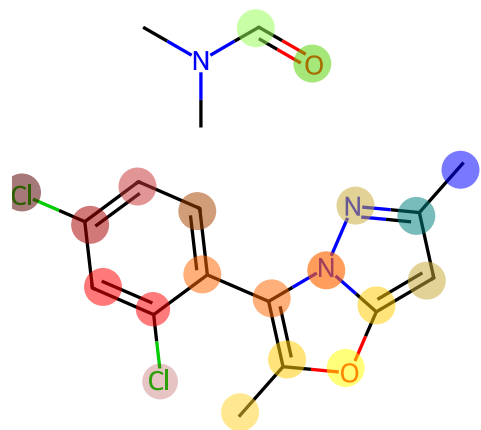


Target (reactants)

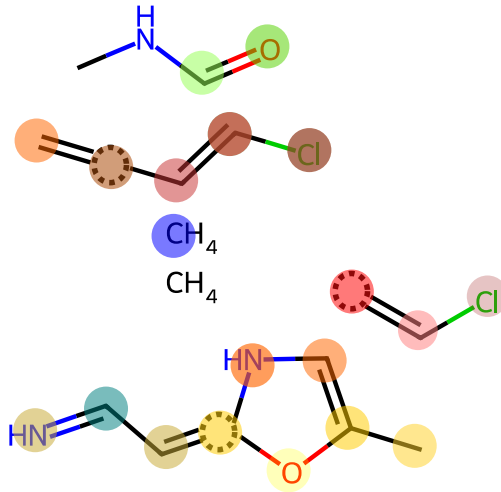


$\mathbf{X}_0$

$$q(\mathbf{X}_{t+1}|\mathbf{X}_t)$$

...

$$p_\theta(\mathbf{X}_t|\mathbf{X}_{t+1}, \mathbf{Y})$$

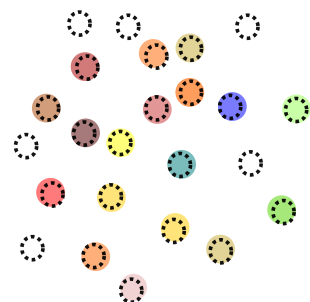


$\mathbf{X}_t$

$$q(\mathbf{X}_t|\mathbf{X}_{t-1})$$

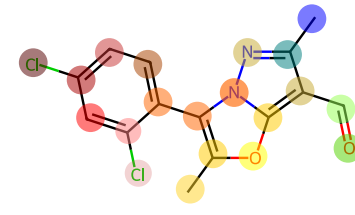
...

$$p_\theta(\mathbf{X}_{t-1}|\mathbf{X}_t, \mathbf{Y})$$



$\mathbf{X}_T$

Input (product)



$\mathbf{Y}$

$$= \sum_{\mathbf{X}_0} q(\mathbf{X}_0|\mathbf{X}_T, \mathbf{X}_0) p_\theta(\mathbf{X}_0|\mathbf{X}_T, \mathbf{Y}, \mathbf{P}^{\mathbf{Y} \rightarrow \mathbf{X}})$$