$$R^{(3)} = R^{(2)} - \frac{E'(R^{(2)})}{E''(R^{(2)})}$$

osv osv.

Generelt: $R^{(n+1)} = R^{(n)} - \dfrac{E'(R^{(n)})}{E''(R^{(n)})}$ $\quad n = 1, 2, \ldots$

inntil $|R^{(n+1)} - R^{(n)}| < \delta$

der δ = konvergenskriterium, f.eks. 0.001 Å

Generalisering til fleratomig molekyl (A atomer):

$$\vec{R}^{(n+1)} = \vec{R}^{(n)} - (\nabla E)^{(n)} \cdot (\mathcal{H}^{(n)})^{-1}$$

$$\vec{R} = (x_1, y_1, z_1, x_2, y_2, z_2, \ldots\ldots, x_A, y_A, z_A) \quad (1 \times 3A) \text{ vektor}$$

$$\nabla E = \left(\frac{\partial E}{\partial x_1}, \frac{\partial E}{\partial y_1}, \frac{\partial E}{\partial z_1}, \ldots\ldots, \frac{\partial E}{\partial z_A}\right) \quad (1 \times 3A) \text{ vektor}$$

$$\mathcal{H} = \begin{pmatrix} \frac{\partial^2 E}{\partial x_1^2} & \frac{\partial^2 E}{\partial x_1 \partial y_1} & \cdots & \frac{\partial^2 E}{\partial x_1 \partial z_A} \\ \vdots & & & \\ \frac{\partial^2 E}{\partial z_A \partial x_1} & \cdots & \cdots & \frac{\partial^2 E}{\partial z_A^2} \end{pmatrix} \quad (3A \times 3A) \text{ matrise}$$

= "2. derivert av energien"-matrisen ("Hessian")

[Kommentar: ∇E og $\mathcal{H}$ beregnes <u>analytisk</u> i mange molekylmodelleringsprogrammer]