It is noteworthy that we do not need to construct the covariant terms for the system (8a). Only their assumed existence was used in (7). But there are in (8a) as well as in (8b) some specific "cliffs" for a numerical computation:

—The g^{kl} in Eq. (8a) are only given as function of x. Hence, from one step to the next it is additionally necessary to use transformation (6).
—Using (8b) and (15) we have to solve a linear system of equations in each step. But the matrix of the coefficients $g_{kl}(q)$ has favorable properties: It is symmetric and positive definite.

The ordinary mathematical device to take over the metric from R^{3N} to R^n is given by Eqs. (6) and (15) using the dependence $g_{kl} = g_{kl}(q)$ to get the inverse $g^{kl} = g^{kl}(q)$ as function of q in Eq. (8a). Then in Eqs. (8a) and (13) we would have to deal with internal coordinates only. But experience shows the possible difficulty of the inversion process. It is hoped that our way of getting (8a) can serve as a good compromise.

(iv) What happens with the degrees of freedom for overall motions? The introduction of the gradient systems (8) involves a two-fold difficulty: Additional to the differential geometrical problems we have to reduce the $3N$ degrees of freedom to $n = (3N-6)$. The crucial point are Eqs. (5) for the backtransformation (6). With $q \to x(q)$ we get from R^n in R^{3N} only a parametric representation of an n-dimensional submanifold, which is fixed by "initial values" (5) somewhere in the R^{3N}. But we do not get the whole R^{3N} itself. In fact we lose a 6-dimensional manifold.

Nevertheless, the system (8) is correct because of the special structure of our problem. We explain this in view of system (5a): We choose n internal coordinates $q^1, \ldots, q^n$ and additional three coordinates for the geometrical center of the molecule with respect to the laboratory origin:

$$q^{n+a} := 1/N \sum_{l=0}^{N-1} x^{a+3l}, \qquad a = 1, 2, 3. \tag{16}$$

Thus contrarily to (5a) we do not constrain the q^{n+a} to 0. We get

$$\frac{\partial q^{n+a}}{\partial x^{b+3l}} = \begin{cases} 1/N & \text{for } a = b, \quad a, b = 1, 2, 3 \\ 0 & \text{for } a \neq b, \quad l = 0, \ldots, N-1. \end{cases} \tag{17}$$

We assume the potential to be independent of the locus in the ordinary 3-dimensional space. Let h be a displacement in any direction, e.g. in the x-direction:

$$U(x^1, \ldots, x^{3N}) = U(x^1 + h, x^2, x^3, x^4 + h, \ldots, x^{3N})$$

thus

$$\frac{\partial U}{\partial h} = 0 = \sum_{l=0}^{N-1} \frac{\partial U}{\partial x^{1+3l}}, \tag{18}$$

and consequently

$$\frac{\partial V}{\partial q^{n+a}} = 0, \qquad a = 1, 2, 3$$

if we take for example

$$q^{n+a} + h = 1/N \sum_{l=0}^{N-1} (x^{a+3l} + h).$$

So the first n equations in the system (8a) have not to be changed. For the three new coordinates we get three additional equations

$$\frac{dq^{n+a}}{dt} = -\sum_{k=1}^{n} g^{(n+a)k} \frac{\partial V}{\partial q^k}, \qquad a = 1, 2, 3. \tag{19}$$

With definition (4) and the particular property (17) the trivial factors $1/N$ or zero are obtained in the new $g^{(n+a)k}$ giving

$$g^{(n+a)k} = 1/N \sum_{l=0}^{N-1} \frac{\partial q^k}{\partial x^{a+3l}}.$$

Now we expand:

$$\sum_{k=1}^{n} \frac{\partial V}{\partial q^k} \left(\frac{1}{N} \sum_{l=0}^{N-1} \frac{\partial q^k}{\partial x^{a+3l}} \right) = \frac{1}{N} \sum_{l=0}^{N-1} \sum_{k=1}^{n} \frac{\partial V}{\partial q^k} \frac{\partial q^k}{\partial x^{a+3l}}$$

$$= \frac{1}{N} \sum_{l=0}^{N-1} \cdot \frac{\partial U}{\partial x^{a+3l}} = 0, \tag{20}$$

where we used the chain rule and Eq. (18). Hence we have in Eq. (19) always

$$\frac{dq^{n+a}}{dt} = 0 \quad \text{for } a = 1, 2, 3.$$

The geometrical centre of the chemical system does not move and we can really cancel the three Eqs. (19) in the system (8a), as we did above.

(v) The use of mass weighted coordinates. Our theorem additionally clarifies the question of using mass weighted coordinates for the path of steepest descent [15, 33, 49, 50]. In system (2) the trivial metric tensor is $g^{ij} = \delta^{ij}$, $i, j = 1, \ldots, 3N$. Now we choose the centre of mass as origin. The transformations

$$Q^i = m_i^{1/2} x^i \quad \text{and} \quad V(Q^i) = U(Q^i / m_i^{1/2}) \tag{21}$$

give the mass weighted Cartesian system Q^i and the transformed potential (m_{a+3l}, $a = 1, 2, 3$; $l = 0, \ldots, N-1$ labelling the $(l+1)$th atomic mass). According to (4) we have

$$g^{kj} = \sum_{i=1}^{3N} m_k^{1/2} \delta^{ki} m_j^{1/2} \delta^{ij} = (m_k m_j)^{1/2} \delta^{kj} = \begin{cases} m_j & \text{for } k = j \\ 0 & \text{for } k \neq j. \end{cases} \tag{22}$$