Transformations Made in VCTrans

In this document the information in the **.info** file is decscribed, giving units and relating it to the information read from a Quantum Chemistry output.

1 General Information

This initial section contains the information read from the **file0**, which contains the geometry around which the VCHam expansion is made, the vibrations, and the Cartesian $\leftrightarrow$ Normal Mode transformation matrices.

1. *zero_of_energy* The zero of energy (in eV) as given in the input file or read from the **file0**. All energies in the data sets are relative to this value.

2. *equilibrium_state_geometry.* The Cartesian coordinates of the expansion point geometry from the *file0* in Å.

3. *masses* Atomic masses in amu.

4. *vibrational_frequencies* The frequencies for the normal modes from **file0**, in eV.

5. normal_modes The normal mode coordinates in terms of the atomic Cartesian coordinates. There are m normal mode vectors with $3N$ components. These vectors are the eigenvectors of the mass-weighted Hessian[1] . How they relate to the Quantum Chemistry output depends on the normal mode definition of the code used. Most codes (Gaussian, Molpro, Molcas, Qchem,...') give the normal modes in non mass-weighted Cartesian coordinates.

2 Normal mode transformation matrices

If the keyword `nmode_trafos` is given in the input file, this section of data is written with the actual transformation matrices as used. There are 2 matrices

1. *forward nm* $\rightarrow$ *coo.* There are m vectors with $3N$ components, as with the normal mode coordinate definition. These are the columns of the matrix that transforms from mass-frequency scaled normal modes to Cartesians in Å.[2]

2. *backward coo* $\rightarrow$ *nm* There are $3N$ vectors with m components. These are the columns of the matrix that transforms from Cartesians in Å to mass-frequency scaled normal modes.[3]

[1] In the notes on "Normal Mode Coordinates" this is the matrix $\mathbf{D}$ in Eqs. (6-8)

[2] In the notes on "Normal Mode Coordinates" this is the matrix $\tilde{\mathbf{D}}'$ in Eq. (19). The transformation is Eq. (17)

[3] In the notes on "Normal Mode Coordinates" this is the matrix $\tilde{\mathbf{D}}$ in Eq. (18). The transformation is Eq. (16)

3 Data Sets

The data sets contain the data taken from each output file in the order defined in the input file. Each data set has the same information. What exactly is included depends on what has been asked for.

1. *point_in_cartesian_coordinates* is the geometry in Å.

2. *point_in_q* is the geometry transformed to mass-frequency scaled normal mode coordinates.
$$\mathbf{q} = \tilde{\mathbf{D}} \left(\mathbf{x} - \mathbf{x}_0 \right) \tag{1}$$
where $\mathbf{x}_0$ is the *equilibrium_state_geometry* and $\tilde{\mathbf{D}}$ the coordinate to normal mode transformation matrix.

3. *gradient* is the potential gradient in Cartesian coordinates in eV/Å.

4. *gradient_in_q* is the gradient transformed to mass-frequency scaled normal mode coordinates.
$$\mathbf{F}_q = \left(\tilde{\mathbf{D}}' \right)^T \mathbf{F}_x \tag{2}$$
where $\mathbf{F}_x$ is the gradient (negative of the force) in Cartesians in eV/Å, $(\tilde{\mathbf{D}}')^T$ is the transpose of the forward nm $\rightarrow$ coo trasformation matrix, and $\mathbf{F}_q$ the gradient in mass-frequency scaled normal modes in eV.

5. *linear_coupling* is the non-adiabatic coupling in eV/Å, $\langle \Phi_i | \frac{\partial H}{\partial x} | \Phi_j \rangle$, between the states i, j which are defined in the following line.

6. *linear_coupling_in_q* is the non-adiabatic coupling in mass-frequency scaled normal modes, in eV, between the same states as the preceeding linear_coupling block. The transformation is as for the gradient_in_q.