Rust INTDER Manual

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INTDER is a program for performing coordinate transformations between simple-/symmetry-internal coordinates and Cartesian coordinates. It was originally written in Fortran by Wesley D. Allen and coworkers but has since been translated to Rust by Brent R. Westbrook. This documentation corresponds to the Rust version only.

1 Internal Coordinates

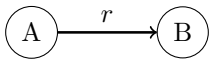
At their most basic, internal coordinates are those defined with reference to other atoms in the same molecule (or system), as opposed to an external set of axes or some other frame of reference. Simple examples of internal coordinates are distances between pairs of atoms and angles between sets of three atoms. A major benefit of using internal coordinates over an external coordinate system like Cartesian coordinates is that internal coordinates require only $3N - 6$ (or $3N - 5$ for linear molecules) coordinates to describe a system fully since the 3 translational and 3 rotational degrees of freedom only have meaning in an external reference frame. N in this case is, of course, the number of atoms in the system. Given the exponential scaling of the number of points required to describe a quartic force field (QFF), or really any potential energy surface (PES), with the number atoms, this difference of 6 coordinates can have a large effect. As a result, using internal coordinates can lead to a substantial decrease in computational cost for such a PES. The types of simple-internal coordinates supported by INTDER are described in the following subsections.

1.1 Simple-Internal Coordinates

1.1.1 Stretch

The bond stretch, referred to as `STRE` in the input file, is the distance between two atoms, as shown in Fig. 1. When the direction matters, the distance is computed from atom `A` to atom `B`, using the equation given in Eqn. 1, where a_i and b_i represent the ith components of the Cartesian coordinates of atoms `A` and `B`, respectively.

Figure 1: A stretch



$$r = \sqrt{\sum_i (b_i - a_i)^2} \tag{1}$$

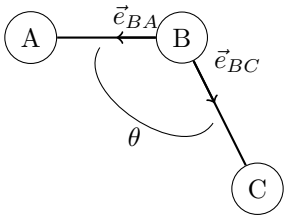
1.1.2 Bend

The bend, referred to as `BEND` in the input file, is the angle between three atoms, as shown in Fig. 2.

The value of the angle, θ is computed using Eqn. 2, where $\vec{e}_{ij}$ represents the unit vector pointing from atom i to atom j.

$$\theta = \text{acos}(\vec{e}_{BA} \cdot \vec{e}_{BC}) \tag{2}$$

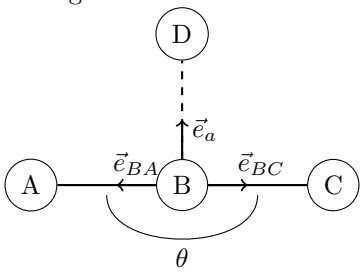
Figure 2: A bend



1.1.3 Linear bend

The linear angle bend, referred to as `LIN1` in the input file, is similar to a regular bend, but atoms `A`, `B`, and `C` are in a line, so specifying the angle between them requires a fourth atom, `D`, which must be a dummy atom specified at the end of the geometry. Typically the coordinates of `D` are chosen to align with the central atom `B` along the axis of the molecule but to project along another axis, as shown in Fig. 3.

Figure 3: A linear bend



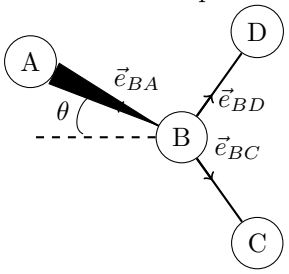
The value of the linear bend is computed using Eqn. 3 where $\vec{e}_a$ is the unit vector in the Cartesian direction of the dummy atom. Nothing in the code actually checks that it aligns with atom `B`, so the caller is responsible for making sure this is the case.

$$\theta = \text{asin}\left(\vec{e}_a \cdot (\vec{e}_{BC} \times \vec{e}_{BA})\right) \tag{3}$$

1.1.4 Out

The out-of-plane bend, referred to as `OUT` in the input file, is the angle between atom `A` and the plane formed by atoms `B`, `C`, and `D`, as shown in Fig. 4.

Figure 4: An out-of-plane bend



The value of θ is computed with the equations below, with the caveat that if $w_1 + w_2$ is greater than zero, the value of theta is set to π with the sign of θ, minus θ.

$$\vec{v}_5 = \vec{e}_{BC} \times \vec{e}_{BD} \tag{4}$$
$$w_1 = \vec{e}_{BA} \cdot \vec{e}_{BC} \tag{5}$$
$$w_2 = \vec{e}_{BA} \cdot \vec{e}_{BD} \tag{6}$$
$$\phi = \sin\left(\operatorname{acos}(\vec{e}_{BC} \cdot \vec{e}_{BD})\right) \tag{7}$$
$$\theta = \operatorname{asin}(\vec{e}_{BA} \cdot \vec{v}_5/\phi) \tag{8}$$

1.1.5 Torsion

The torsional angle, referred to as `TORS` in the input file, is the angle between the planes formed by the overlapping sets of atoms `A`, `B`, `C`, and `B`, `C`, `D`, as shown in Fig. 5. Vectors $\vec{v}_5$ and $\vec{v}_6$ are the vectors normal to the planes ABC and BCD, respectively, found by $\vec{e}_{BA} \times \vec{e}_{CB}$ and $\vec{e}_{DC} \times \vec{e}_{CB}$. To find the angle θ between these two normals, and thus between the planes, perform the following transformations:

$$w_2 = \vec{e}_{BA} \cdot \vec{e}_{CB} \tag{9}$$
$$w_3 = \vec{e}_{DC} \cdot \vec{e}_{CB} \tag{10}$$
$$s_2 = \sqrt{1 - w_2^2} \tag{11}$$
$$s_3 = \sqrt{1 - w_3^2} \tag{12}$$
$$w_4 = \vec{e}_{BA} \cdot \vec{v}_6 \tag{13}$$
$$w_5 = -\vec{v}_5 \cdot \vec{v}_6 \tag{14}$$
$$w = \frac{w_2}{s_2 s_3} \tag{15}$$
$$\theta_0 = \operatorname{asin} w \tag{16}$$
$$\theta = \begin{cases} \theta_0 & w_3 \geq 0 \\ \pi - \theta_0 & w_3 < 0 \end{cases} \tag{17}$$

Figure 5: A torsion