transfer.nb *

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Mathematica Noteook for Calculating Rate of Excitation Transfer between two BChls

NOTE: To execute a group of command lines, click anywhere within a cell covered by a blue bracket on the right which has a semi-arrow, press and hold the Shift key and then press Enter.

■ 1. Define constants and Load a package called "VectorAnalysis".

```
const := 505644; (* unit is angstrom cube per cm *)
hbar := 6.582*10^-16 *8065.82*10^12 ; (* equal to 5.3089 ps per cm *)
J := 10.5*10^-4; (* Unit in cm *)
J1 := 2.705*10^-4;
J2 := 6.295*10^-4;
<< Calculus`VectorAnalysis`
```

■ 2. Compute the directional vector d1 of the transition dipole moment of BChl B850a (red, Segname BCA1, ResID 59)

```
rNB1 = {19.582, -14.681, 71.801};
rNB1 = {15.852, -16.009, 72.315};
B1 = rNB1 - rNB1;
B1sq = DotProduct[B1, B1];
d1 = B1 / Sqrt[B1sq]
```

{-0.927685, -0.350258, 0.127864}

■ 3. Compute the directional vector d3 of the transitiom dipole moment of BChl B850a (red, Segname BCA2, ResID 59)

```
rNB3 = {24.171, 3.522, 71.801};
rNB3 = {22.529, -0.111, 72.315};
B3 = rNB3 - rNB3;
B3sq = DotProduct[B3, B3];
d3 = B3 / Sqrt[B3sq]
```

{-0.480475, -0.903769, 0.127866}

```
rMG1 = {rMG1x, rMG1y, 72.084};
```

■ 4. Compute the separation distance between the two central Mg2+ ions (Segment BCA1 and BCA2, Name MG and ResID 59)

```
rMG1 = {17.758, -15.464, 72.084};
rMG1 = {23.406, 1.616, 72.084};
```