Computation of torsional angle

Torsion angle: It is angle defined between two planes such that both planes share a common vector defining the planes. Consider four connected atoms A-B-C-D (see figure 1).

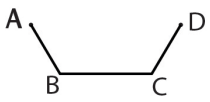
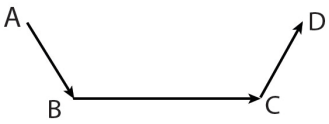
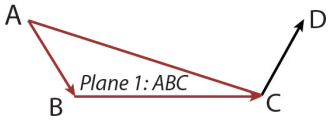
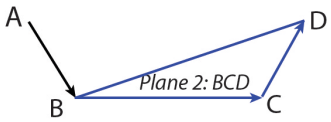


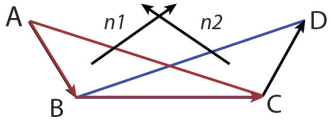
Figure 1

Figure 2









Two planes are defined as described as given below:

- Plane 1: ABC defined by normal (n1) given by vectors A-B and B-C
- Plane 2: BCD defined by normal (n2) given by vectors B-C and C-D. Note: The B-C vector is common to both planes ABC and BCD

The angle between these two planes is computed using dot product of their normal. Following the IUPAC nomenclature, the sign is defined by taking the dot product of cross product of two normal (n1 x n2) and BC vector. If the dot product is negative, the angle is defined as negative, otherwise it is positive.

Phi angle: C(i-1)-N(i)-CA(i)-C(i)
Psi angle: N(i)-CA(i)-C(i)-N(i+1)

Algorithm steps:

v1 is vector (AB)

v2 is vector (BC)

v3 is vector (CD)

n1 = v1 X v2 (Cross Product)

n2 = v2 X v3 (Cross Product)

The angle between n1 and n2 is obtained by:

$$angle = \cos^{-1}\frac{n1.n2}{|n1||n2|}$$

Sign of angle is given by:

Sign=+1

n12 = n1 X n2 (Cross Product)

value = n12.v2 (dot product)

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If the value < 0:
    Sign=Sign*-1
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Cross product is defined as below:

$$\vec{Y} = xi + yj + zk$$

$$\vec{Y} = ai + bj + ck$$

$$\vec{X}\times\vec{Y} = (yc - zb)i + (za - xc)j + (xb - ya)k$$