Example of a command (.com) file and description of a geometry with a **Z-matrix**

```
#N HF/3-21G OPT

H2O2

0 1
O
O 1 B1
H 2 B2 1 A1
H 1 B3 2 A2 3 D1

B1 1.4600000
B2 1.0500000
B3 1.0500000
A1 109.47122
A2 109.47122
D1 180.00000
```

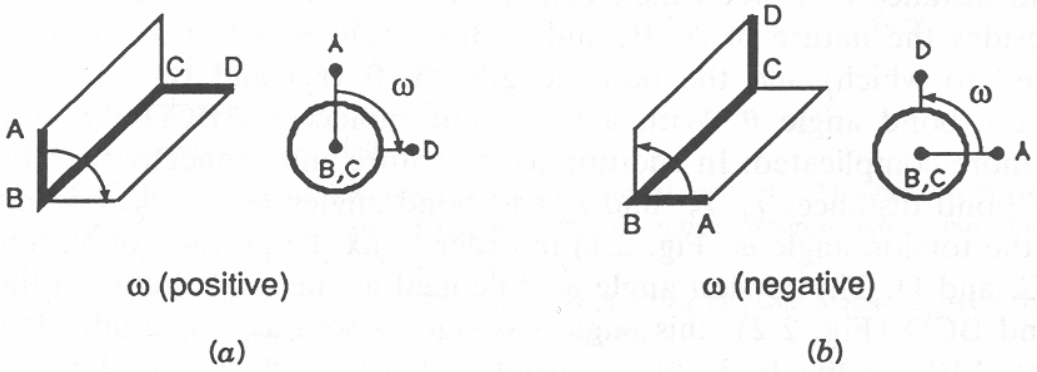

Figure 2.2. Torsion angle.

TABLE 2.2. Specification of Torsion Angle (Klyne–Prelog).

Angle of Torsion (ω)	Designation	Symbol
−30 to +30°	synperiplanar	sp^a
+30 to +90°	+ synclinal	$+sc^b$
+90 to +150°	+ anticlinal	$+ac$
+150 to −150°	antiperiplanar	ap^c
−150 to −90°	− anticlinal	$-ac$
−90 to −30°	− synclinal	$-sc^b$

[a] The designation syn or eclipsed are often used for $\omega \approx 0°$.
[b] The designation gauche is frequently used for $\omega \approx 60°$.
[c] The designation anti (or, less properly, trans) is often used for $\omega \approx 180°$.

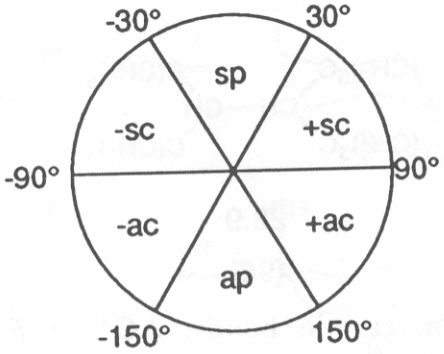

Figure 2.13. Specification of torsion angle (Klyne–Prelog).

From *Stereochemistry of Organic Compounds*, Ernest L. Eliel and Samuel H. Wilen, New York, Wiley, 1994.