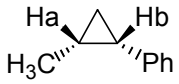
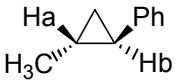
几种常见结构相邻碳上氢（Ha-C-C-Hb）的偶合常数

偶合常数和化学位移一样，是鉴定有机化合物分子结构的一个重要数据。偶合常数起源于自旋的核之间的相互干扰，其大小与外加磁场大小无关。自旋的核之间的相互干扰，是通过它们之间的键上成键电子传递的，所以偶合常数的大小主要与它们之间键的数目有关，也与影响它们之间电子云分布的因素（如单键、双键、取代基的电负性、立体化学等）有关。所以某些有机化合物的顺反结构可以通过偶合常数的大小判断。

环丙烷类化合物：顺式结构的偶合常数一般大于反式结构。顺式时偶合常数在 7-11 Hz 之间；反式时偶合常数在 4.5-7.5 Hz 之间。举例如下：



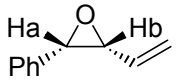


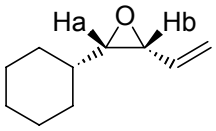
Ha, δ = 0.97；Hb, δ = 2.07；　Ha, δ = 0.87；Hb, δ = 1.56；

顺式：J_{ab} = 8.5 Hz　　反式：J_{ab} = 5.0 Hz

J. Am. Chem. Soc. **1979**, *101*, 7982

环氧乙烷类化合物：该类化合物与环丙烷类化合物类似，其顺式结构的偶合常数一般大于反式结构。顺式时偶合常数在 3.5-5 Hz 之间；反式时偶合常数在 2-4 Hz 之间。举例如下：

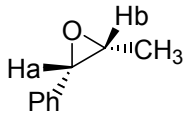


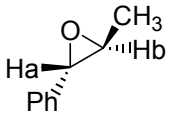


Ha, δ = 4.25；Hb, δ = 3.67；　Ha, δ = 2.77；Hb, δ = 3.39；

顺式：J_{ab} = 4.1 Hz　　顺式：J_{ab} = 4.4 Hz

J. Org. Chem. **1996**, *61*, 7513



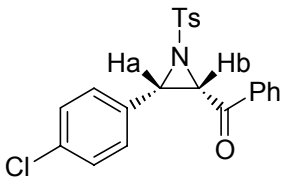


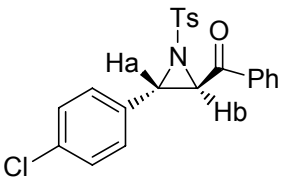
Ha, δ = 4.07；Hb,δ =3.35；　Ha, δ = 3.58；Hb, δ = 3.04；

顺式：J_{ab} = 4.4 Hz　　反式：J_{ab} = 2.2 Hz

Tetrahedron. **1994**, *50*, 11827

氮杂环丙烷类化合物：该类化合物与环丙烷类化合物类似，其顺式结构的偶合常数一般大于反式结构。

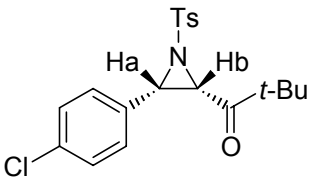


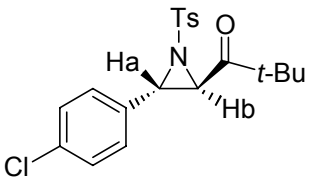


Ha,δ = 4.30；Hb,δ = 4.41；　Ha,δ = 4.24；Hb, δ = 4.48；

顺式：J_{ab} = 7.5 Hz　　反式：J_{ab} = 4.3 Hz

J. Org. Chem. **1995**, *60*, 4665



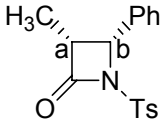


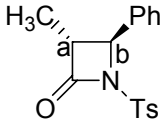
Ha,δ = 4.06；Hb,δ = 4.14；　　Ha,δ = 3.93；Hb,δ = 4.25；

顺式：J_{ab} = 7.6 Hz　　反式：J_{ab} = 4.1 Hz

J. Org. Chem. **1995**, *60*, 4665

四元环类化合物：顺式结构的偶合常数一般大于反式结构。

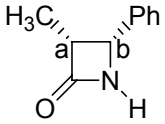


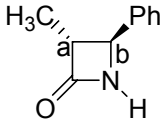


Ha,δ = 3.60；Hb,δ = 5.22；　　Ha,δ = 3.16；Hb,δ = 4.60；

顺式：J_{ab} = 6.7 Hz　　反式：J_{ab} = 3.1 Hz

Tetrahedron. **1994**, *50,* 12755



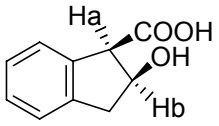


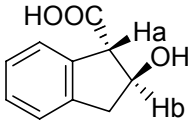
Ha,δ = 3.57；Hb,δ = 4.88；　　Ha,δ = 3.06；Hb,δ = 4.31；

顺式：J_{ab} = 5 Hz　　反式：J_{ab} = 2 Hz

Tetrahedron. **1994**, *50,* 12755

环戊烷类化合物：顺式结构和反式结构的偶合常数一般差别不大。顺式时偶合常数在 4-5 Hz 之间；反式时偶合常数也在 4-5 Hz 之间。举例如下：



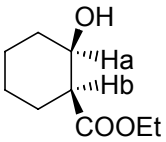


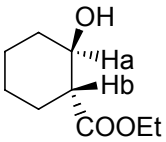
Ha,δ = 3.97；Hb,δ = 4.70；　　Ha,δ = 3.75；Hb,δ = 4.65；

顺式：J_{ab} = 5 Hz　　反式：J_{ab} = 5 Hz

Tetrahedron. **1991**, *47*, 4941

环己烷类化合物：a, a 的偶合常数在 8-12 Hz 之间；a, e 和 e, e 的偶合常数在 2-7 Hz 之间。举例如下：



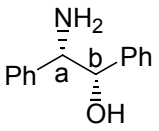


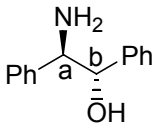
Ha,δ = 3.20；Hb,δ = 2.48；　　Ha,δ = 2.83；Hb,δ = 2.25；

顺式：J_{ab} = 2.6 Hz　　反式：J_{ab} = 3.7 Hz

Tetrahedron. **2000**, *56,* 5639

几个常见的非环状结构的例子：

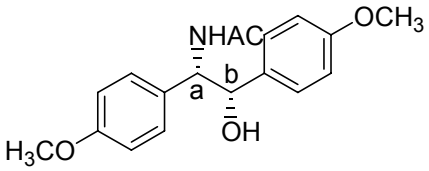


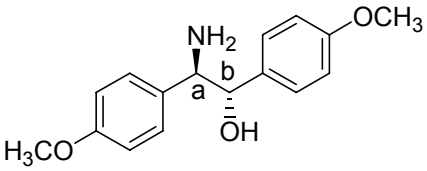


Ha,δ = 3.95；Hb,δ = 4.61；
顺式：J_{ab} = 6.6 Hz

Ha,δ = 4.13；Hb,δ = 4.71；
反式：J_{ab} = 6.3 Hz

Tetrahedron. **1998**, *54,* 10265

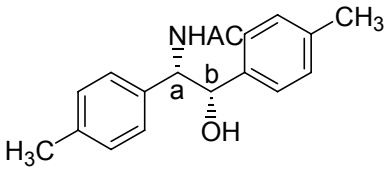


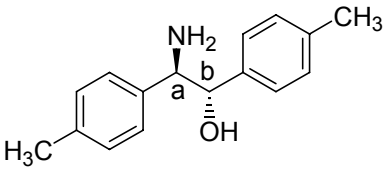


Ha,δ = 4.17；Hb,δ = 5.95；
顺式：J_{ab} = 9.24 Hz

Ha,δ = 4.06；Hb,δ = 4.63；
反式：J_{ab} = 6.41 Hz

Tetrahedron. **1998**, *54,* 10265





Ha,δ = 4.93；Hb,δ = 5.18；
顺式：J_{ab} = 4.62 Hz

Ha,δ = 4.08；Hb,δ = 4.80；
反式：J_{ab} = 6.71 Hz

Tetrahedron. **1998**, *54,* 10265