

## 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,  $\delta = 0.97$ ; Hb,  $\delta = 2.07$ ;    Ha,  $\delta = 0.87$ ; Hb,  $\delta = 1.56$ ;  
 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,  $\delta = 4.25$ ; Hb,  $\delta = 3.67$ ;    Ha,  $\delta = 2.77$ ; Hb,  $\delta = 3.39$ ;  
 顺式:  $J_{ab} = 4.1$  Hz                      顺式:  $J_{ab} = 4.4$  Hz

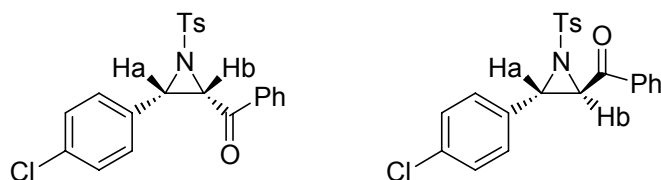
*J. Org. Chem.* **1996**, *61*, 7513



Ha,  $\delta = 4.07$ ; Hb,  $\delta = 3.35$ ;    Ha,  $\delta = 3.58$ ; Hb,  $\delta = 3.04$ ;  
 顺式:  $J_{ab} = 4.4$  Hz                      反式:  $J_{ab} = 2.2$  Hz

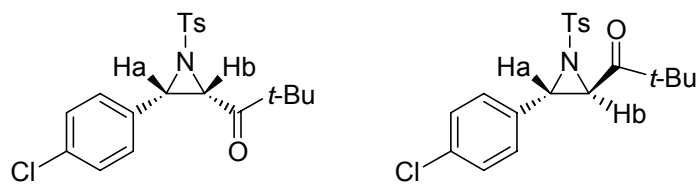
*Tetrahedron.* **1994**, *50*, 11827

**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,  $\delta = 4.30$ ; Hb,  $\delta = 4.41$ ;    Ha,  $\delta = 4.24$ ; Hb,  $\delta = 4.48$ ;  
 顺式:  $J_{ab} = 7.5$  Hz                      反式:  $J_{ab} = 4.3$  Hz

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



Ha,  $\delta$  = 4.06; Hb,  $\delta$  = 4.14;

Ha,  $\delta$  = 3.93; Hb,  $\delta$  = 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,  $\delta$  = 3.60; Hb,  $\delta$  = 5.22;

Ha,  $\delta$  = 3.16; Hb,  $\delta$  = 4.60;

顺式:  $J_{ab}$  = 6.7 Hz

反式:  $J_{ab}$  = 3.1 Hz

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



Ha,  $\delta$  = 3.57; Hb,  $\delta$  = 4.88;

Ha,  $\delta$  = 3.06; Hb,  $\delta$  = 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,  $\delta$  = 3.97; Hb,  $\delta$  = 4.70;

Ha,  $\delta$  = 3.75; Hb,  $\delta$  = 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,  $\delta$  = 3.20; Hb,  $\delta$  = 2.48;

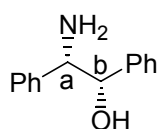
Ha,  $\delta$  = 2.83; Hb,  $\delta$  = 2.25;

顺式:  $J_{ab}$  = 2.6 Hz

反式:  $J_{ab}$  = 3.7 Hz

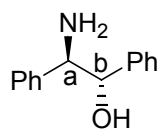
*Tetrahedron.* **2000**, *56*, 5639

几个常见的非环状结构的例子:



Ha,  $\delta$  = 3.95; Hb,  $\delta$  = 4.61;

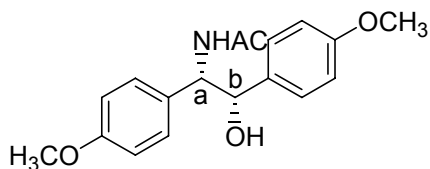
顺式:  $J_{ab}$  = 6.6 Hz



Ha,  $\delta$  = 4.13; Hb,  $\delta$  = 4.71;

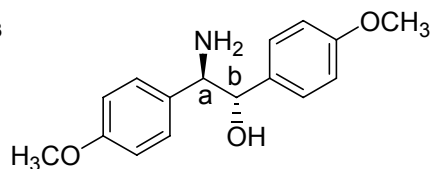
反式:  $J_{ab}$  = 6.3 Hz

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



Ha,  $\delta$  = 4.17; Hb,  $\delta$  = 5.95;

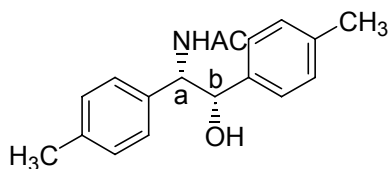
顺式:  $J_{ab}$  = 9.24 Hz



Ha,  $\delta$  = 4.06; Hb,  $\delta$  = 4.63;

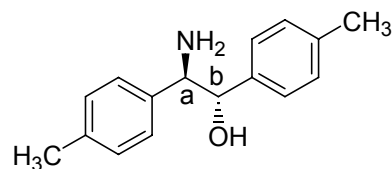
反式:  $J_{ab}$  = 6.41 Hz

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



Ha,  $\delta$  = 4.93; Hb,  $\delta$  = 5.18;

顺式:  $J_{ab}$  = 4.62 Hz



Ha,  $\delta$  = 4.08; Hb,  $\delta$  = 4.80;

反式:  $J_{ab}$  = 6.71 Hz

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