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重水中固氮酶催化还原乙炔产物的^1H NMR研究

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摘要 用^1HNMR研究了固氮酶在重水中催化还原乙炔的反应产物氘代乙烯.
种用群对称性对^1HNMR谱图进行了归属,计算了几种可能的C`2H~2D~2
结构以及C~2H~3D结构的NMR谱线频和强度,得出了理论谱.通过理论谱与实验谱的比较,
表明固氮酶在重水中催化还原乙炔的产物主要以顺式结构C~2H~2D~2为主,并含有较多的单氘代烯.
单氘代乙烯相对乙烯的化学位移往高场移动约4.0Hz,而双氘代乙烯向高场的位移大约是单氘代乙烯的2倍左右。

关键词 乙炔 氘代乙烯 催化反应 固氮酶 重水 化学位移 质子磁共振谱法

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^1H NMR study on the products of the catalytic reduction of ethyne by nitrogenase in D~2O

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Abstract The products of the catalytic reduction ethyne by nitrogenase in D~2O were studied by ^1H NMR. In order to assign the ^1H NMR spectrum, the theoretical spectra of C~2H~2D~2 were calculated using group symmetry. The final eigenfunctions,eigenvalues,allowed transitions and intensities of C~2H~2D~2 and C~2H~2D were obtained.It can be concluded that the products comprised mainly of cis-C~2H~2D~2.There was also some C~2H~3D. ^1H chemical shift in C~2H~3D moved by ca.4. 0Hz to the upfield compared with that in C~2H~4. The upfield shift in C~2H~2D~2 was about twice as large as that in C~2H~3D. The theorical results are in good agreement with experimental ones.

Key words ACETYLENE CATALYTIC REACTION NITROGENASE HEAVY WATER CHEMICAL SHIFT PROTON MAGNETIC RESONANCE SPECTROMETRY

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