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^{13}C NMR Spectroscopy: A Tool for Study of Conformational Analysis of 2-Aryl-*trans*-decahydroquinolin-4-ols

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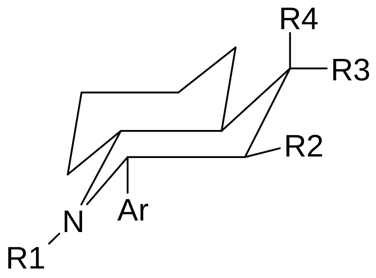
Abstract:

In this investigation, proton decoupled ^{13}C NMR Spectroscopy was used as a tool for the study of conformations of differently substituted 2-aryl-*trans*-decahydroquinolin-4-ols. The fusion of the rings in 2-aryl-*trans*-decahydroquinolin-4-ols was conclusively proved to be *trans*-, from a comparison of the experimental and calculated values. The signal assignments were made on the basis of the model system and in this case *trans*- decahydroquinoline was taken as model system. Substituent parameters for methyl, hydroxyl, and phenyl groups were derived from analogous systems and incorporated in the model system to obtain the calculated values. An examination of the ^{13}C chemical shift values indicated that the configuration of the hydroxyl group was equatorial in all the *α*- forms of 2-aryl-*trans*-decahydroquinolin-4-ols and that of *β*-form's was axial. In 3-Methyl-2-aryl-*trans*-decahydroquinolin-4-ols the chemical shifts suggested equatorial configuration to methyl and phenyl groups. Further, for 1-Methyl-2-aryl-*trans*-decahydroquinolin-4-ol and 1,3-dimethyl-2-aryl-*trans*-decahydroquinolin-4-ols the 1- or N-methyl group was found to has a greater preference to the equatorial position.

Keywords: Decahydroquinolines, conformational analysis, ^{13}C NMR Spectroscopy.

Introduction:

Stereochemical problems were increasingly being investigated by ^{13}C nuclear magnetic resonance techniques[1-3]. The chemical shift values constitute a very sensitive probe for conformational properties. The ^{13}C NMR spectra of a number of cyclohexane[4-7], piperidine[8-11] and decahydroquinolin[12,13] derivatives were recorded and analyzed the conformation and configuration of these systems. A survey of the literature revealed that the ^{13}C NMR spectra of 2-aryl-decahydroquinolin systems were not recorded for the study of conformational analysis. As a part of our extension studies in respect of decahydroquinolin-4-ons/4-ols[14-20] the present investigation involving the study of conformational aspects, the proton decoupled ^{13}C NMR spectra of synthesized 2-aryl-*trans*-decahydroquiolin-4-ols (Fig. 1) (**1-20**) were recorded and an attempt was made to study the configuration and conformations of these compounds.



	Ar	R1	R2	R3	R4
1	C_6H_5	H	H	H	OH
2	C_6H_5	H	H	OH	H
3	*p*-$CH_3.C_6H_4$	H	H	H	OH
4	*p*-$CH_3.C_6H_4$	H	H	OH	H
5	*o*-$Cl.C_6H_4$	H	H	H	OH
6	*o*-$Cl.C_6H_4$	H	H	OH	H
7	*p*-$CH_3O.C_6H_4$	H	H	H	OH
8	*p*-$CH_3O.C_6H_4$	H	H	OH	H
9	C_6H_5	H	CH_3	H	OH
10	C_6H_5	H	CH_3	OH	H
11	*p*-$CH_3.C_6H_4$	H	CH_3	H	OH
12	*p*-$CH_3.C_6H_4$	H	CH_3	OH	H
13	*p*-$Cl.C_6H_4$	H	CH_3	H	OH
14	*p*-$Cl.C_6H_4$	H	CH_3	OH	H
15	*p*-$CH_3O.C_6H_4$	H	CH_3	H	OH
16	*p*-$CH_3O.C_6H_4$	H	CH_3	OH	H
17	C_6H_5	CH_3	H	H	OH
18	C_6H_5	CH_3	H	OH	H
19	C_6H_5	CH_3	CH_3	H	OH
20	C_6H_5	CH_3	CH_3	OH	H

Fig. 1: Substituted 2-aryl-*trans*-decahydroquinolin-4-ols

Materials and Methods

All the compounds were prepared by using known methods and confirmed with the physical constants and spectral data as per literature. Proton decoupled ^{13}C NMR spectra were recorded at 75 MHz on an XLAA 300 (15) spectrometer with a Nicolett TT - 100 Fourier Transform accessory, with TMS as internal standard. $CDCl_3$ was used as a solvent for the majority of the compounds and $CDCl_3$ + DMSO-d6 was used when the compound was not soluble in $CDCl_3$.

Results and Discussion

The 2-aryl-decahydroquiolin-4-ols have either *cis*-or *trans*-form. In this case, even *cis*-form was also considered to be highly stable because of the anchoring effect of phenyl group which exclusively occupied the equatorial position. To solve the problem of ring fusion in the system under investigation, both *cis*- and *trans*-decahydroquinolines were chosen as models and by adding the empirical substituent parameters, the calculated shift values for various carbons for 2-aryl-decahydroquinolin-4-ols were obtained. The values along with the observed shift values revealed that the calculated values, obtained by considering ring fusion to be *trans*-were in good agreement with the determined values. Hence, the ring fusion in 2-aryl-decahydroquinolin-4-ols might considered to be *trans*.

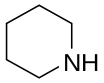
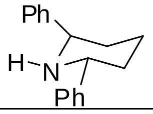
In order to assign the signal positions to various carbon atoms, it is necessary to select some suitable model compounds. Starting from the chemical shift values for the model systems and by adding *α, β* and *γ-gauche* parameters for various substituent's, it is often possible to arrive at the calculated chemical shifts for comparison with those obtained experimentally. In the present investigation two model systems, that is *cis*-and *trans*-decahydroquinolines were chosen. Other model systems were piperidine, 2,6-diphenylpiperidine, and 2,6-diphenylpiperidine-4-ols. Chemical shift parameters for hydroxyl, methyl, and phenyl groups were derived from these model compounds and are given in the following lines.

^{13}C chemical shift parameters for phenyl group:

Chen and Le Fevre[7], from proton NMR studies on phenyl substituted piperidinols observed that the phenyl groups occupy equitorial position. Further, Pandiarajan *et al*[21] observed that phenyl groups in 2,6-diphenylpiperidine-4-ones generally occupy an equatorial position with piperidine chair conformation. This was justified on the grounds that the bulky phenyl groups occupied equatorial position in many systems.

Comparison of the chemical shift values of piperidin **(21)** and 2, 6-diphenylpiperidine **(22)** (**Table 1**), it might be noted that an equatorial phenyl group deshielded the carbon bearing phenyl group by 14.6 ppm and that of *β*- carbon atom by 6.8 ppm. The effect on the *γ*- carbon atom was negligible and the shielding effect of 0.4 ppm was observed.

Table 1: ^{13}C chemical shifts for piperidine and 2,6-diphenylpiperidine

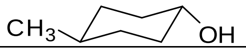
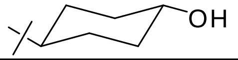
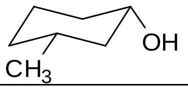
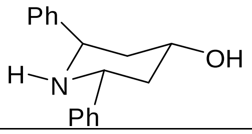
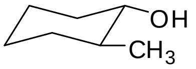
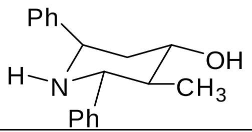
Compd. No	compound	C_2	C_3	C_4
21		47.9	27.9	26.2
22		62.5	34.7	25.8

However, in the absence of a model in which a phenyl group was present in the decahydroquinolin system, the shift parameters obtained from the analogous 2,6-diphenyl piperidine system were considered to be reasonable and hence used for the calculation of the chemical shift values in the present series of compounds.

***^{13}C Chemical shift parameters for hydroxy group*:**

An examination of **Table 2**, indicated that an equatorial hydroxyl group deshielded the α-carbon by 43.7 ± 0.7 ppm, when there was no substituent on the adjacent carbon **(23, 24, 25, and 26)**. The shielding influence of an equatorial hydroxyl group markedly decreased by the steric crowding about the hydroxyl group as evidenced by values observed for **27** and **28**.

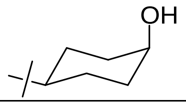
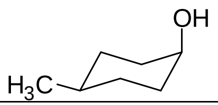
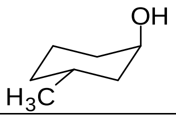
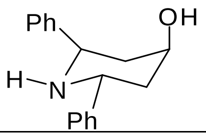
Table 2: Effect (ppm)[a] of an equatorial hydroxyl group on the ring carbon chemical shifts.

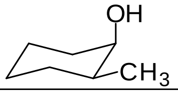
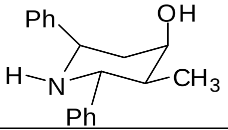
S.No.	compound	α	β	Γ
23		43.0	8.0	-2.8
24		43.2	7.9	-2.5
25		43.7	8.1(c$_2$) 7.7 (c$_6$)	-1.5(c$_3$) -2.4(c$_5$)
26		44.1	9.0	-2.5
27		40.7	6.5(c$_2$) 8.3(c$_6$)	-1.9(c$_3$) -1.3(c$_5$)
28		39.8	7.8(c$_3$) 9.1(c$_5$)	-2.7(c$_2$) -2.6(c$_6$)

In fact, Pandiarajan and Manimekalai[22], while making these observations, concluded that the magnitude and even the sign of the *α*-effect was modified by the presence of a vicinal substituent and ascribed to the presence of *gauche* interaction between the substituent and hydroxyl group. However, the *β*-effects were not significantly modified and the magnitude of *γ*-effect was almost independent of the nearby substituents. Considering the methylene group at C-5 in 2-*aryl*-decahydroquinolin-4-ols to behave like a methyl group (*gauche* to equatorial hydroxyl at C-4) the system might be considered to be similar to 3-methyl-2, 6-diphenylpiperidin-4-ols **(28),** and hence, the shift parameters for an equatorially oriented hydroxyl group were taken from the model system (**28**).

The axial hydroxyl group was expected to deshield the carbinol carbon to a lesser extent than an equatorial hydroxyl group. The observed values at a higher field at around 39.1± 1.3 ppm (α-effect), for an axial hydroxy group when there was no substituent on the adjacent carbon atom, also supported the above comment **(29, 30, 31, 32** in **Table 3).**

Table 3: Effect (ppm) of an axial hydroxyl group on the ring carbon chemical shifts.

S.No.	Compound	A	β	Γ
29		37.8	5.5	-7.2
30		39.2	4.6	-7.2
31		39.7	5.3(c$_2$) 6.1(c$_6$)	-6.6(c$_3$) -6.6(c$_5$)
32		40.3	6.7	-6.5

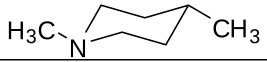
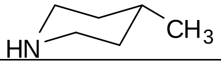
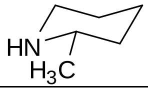
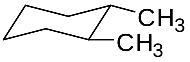
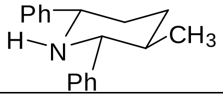
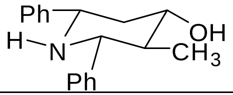
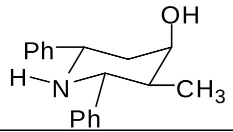
33		35.2	2.6(c_2) 5.0(c_6)	-6.6(c_3) -5.2(c_5)
34		35.0	5.3(c_3) 6.6(c_5)	-7.7(c_2) -7.0(c_6)

The *α*-effect, in this case, was also significantly reduced by a nearby substituent **(33 and 34)**. However, the *β*-and *γ*-effects were not modified to any greater extent as was seen from **Table 3**. Hence, it was considered that the shift parameters in respect of an axially oriented hydroxyl can be taken for those reported for 3-methyl-2,6-diphenylpiperidine-4-ol **(34).**

^{13}C Chemical shift parameters for methyl group:

From **Table 4**, it might be noted that an equatorial methyl group causes a downfield shift of 5.7 ± 0.6 ppm on the methyl group bearing carbon atom when there was no vicinal substituent **(35, 36, 37,** and **38)**.

Table 4: Effect (ppm)^a of an equatorial methyl group on the ring carbon chemical shifts.

S.No.	**Compound**	**A**	**β**	**Γ**
35		5.7	8.6	-0.2
36		6.3	7.3	-0.9
37		5.9	8.7	-0.5
38		5.2	8.2	-0.4
39		3.9	6.8(c_2) 9.1(c_4)	+0.4(c_3) +0.4(c_5)
40		2.7	7.6(c_2) 9.7(c_4)	+0.2
28		1.5	7.4(c_2) 5.4(c_4)	+0.3
34		1.3	6.4(c_2) 4.4(c_4)	+0.1

However, the effect was significantly modified by a vicinal substituent **(39, 40)** and the α-effect was still lower in compounds where there were more nearby substituents **(28, 34).** Further, the β and γ-effects of the methyl group were not modified significantly.

The *α, β,* and *γ*-parameters in respect of an equatorial methyl group reported by Pandiarajan and Manimekalai[22] were taken for calculating the chemical shift values for various carbons in 3-methyl-2-*aryl*-decahydroquinolin-4-ols **(9 to 16)**. The various shift parameters derived for hydroxyl, phenyl, and methyl groups were given in **Table 5**.

Table 5:- Calculated ^{13}C NMR chemical shift parameters

Substituent	α	Β	Γ
Equitorial hydroxyl	39.8	7.8(C-10) 9.1(C-3)	-2.7(C-9) -2.6(C-2)
Axial hydroxyl	35.0	5.3(C-10) 6.6(C-3)	-7.7(C-2) -7.0(C-2)
Equitorial phenyl	14.6	6.8	-0.4
Equitorial methyl (with-OH equatorial)	1.5	7.4(C-2) 5.4(C-4)	+0.3
Equitorialmethyl (with-OH axial)	1.3	6.4(C-2) 4.4(C-4)	+0.1

As mentioned earlier 2-*aryl*-decahydroquinolin-4-ols prepared might exist either in *cis*- or *trans*- form. In this case, even the *cis*- form was considered to be highly stable because of the anchoring effect of a phenyl group, which exclusively occupied equatorial position. In order to solve the problem of ring fusion in the system under investigation, both *cis*- and *trans*-decahydroquinolines were chosen as models and by adding the empirical substituent parameters, the calculated shift values for various carbon atoms for 2-*aryl*-decahydroquinolin-4-ols (**Fig. 1**) were obtained. The values along with the observed shift values were tabulated in **Table 6**.

Table 6: ^{13}C Chemical shifts for 2-aryldecahydroquinolin-4-ols*

Compound	C2	C3	C4	C5	C6	C7	C8	C9	C10	Aromatic Carbons
1	59.6	43.8	73.9	27.5	25.7	25.1	33.2	59.6	49.7	126.7
										127.2
										128.4
										143.9
Trans-	(59.3)	(43.3)	(71.9)	(30.0)	(26.3)	(25.6)	(34.0)	(59.4)	(51.1)	
Cis-	(58.8)	(38.4)	(69.6)	(23.4)	(26.1)	(21.2)	(32.5)	(51.4)	(43.6)	
2	54.6	42.6	67.6	24.7	27.3	25.8	33.4	54.1	46.2	126.4
										127.3
										128.1
										145.6
Trans-	(54.2)	(40.7)	(67.1)	(24.9)	(26.3)	(25.6)	(34.0)	(54.7)	(48.6)	
Cis-	(53.7)	(35.9)	(64.9)	(18.3)	(26.1)	(21.2)	(32.5)	(47.6)	(41.1)	
3	59.6	43.8	74.0	27.5	25.6	25.1	33.1	59.3	49.7	126.1
										126.6
										129.1
										136.0
										141.0
Trans-	(59.3)	(43.3)	(71.9)	(29.9)	(26.3)	(25.6)	(34.0)	(59.5)	(51.1)	
4	53.3	--	66.7	24.9	26.4	--	--	53.2	--	127.5
										125.3

Trans-	(54.2)	(40.7)	(67.1)	(24.9)	(26.3)	(25.6)	(34.0)	(54.6)	(48.6)	
5	55.1	42.0	73.9	27.5	25.9	25.1	33.2	59.5	49.6	127.0
									128.0
									128.5
									129.9
									132.6
									141.1
Trans-	(59.3)	(43.3)	(71.9)	(30.0)	(26.3)	(25.6)	(34.0)	(59.4)	(51.1)	
Compound	C2	C3	C4	C5	C6	C7	C8	C9	C10	Aromatic Carbons
6	51.4	40.6	69.2	24.9	27.5	--	33.8	54.8	46.3	127.1
									127.7
									127.9
									129.3
									132.8
									141.7
Trans-	(54.2)	(40.7)	(67.1)	(24.9)	(26.3)	(25.6)	(34.0)	(54.7)	(48.6)	
7	59.6	43.8	73.9	27.5	25.6	25.1	33.1	59.0	49.6	113.7
									127.7
									136.2
									158.7
Trans-	(59.2)	(43.2)	(71.9)	(29.9)	(26.3)	(25.6)	(34.0)	(59.5)	(51.1)	
8	54.8	42.4	69.4	24.9	27.4	25.1	33.7	54.1	46.2	113.7
									127.8
									136.2
									158.7
Trans-	(54.2)	(40.7)	(67.1)	(24.9)	(26.3)	(25.6)	(34.0)	(54.6)	(48.6)	

** - Values given in parentheses are calculated values.**- The chemical shifts for all carbons could not be recorded because of the poor solubility of the compound.*

An examination of the shift values revealed that the calculated values, obtained by considering the ring fusion to be *trans-*, were in good agreement with the observed values. Hence, the ring fusion in 2-*aryl*-decahydroquinolin-4-ols might reasonably considered to be *trans*. The presence of high field signals (below 25 ppm) was reported to be characteristic in decahydroquinolins with *cis*-fusion[12-13]. The absence of such signals in the compounds now under investigation also supported the *trans*-fusion of the rings. The studies on kinetics of semicarbazone[23] formation also observed that the fusion of the rings in decahydroquinolin-4-ones to be *trans*.

An examination of the values in Table 6, indicated that the observed signal positions were quite frequently agreeing with those of the calculated values within 1 PPM. The difference of about $\Delta\delta$ 2.5ppm was observed for C-5 with an equatorial hydroxy might also be diagnostic as this deviation between the observed and calculated values was not observed in those compounds with axial hydroxy group. This difference might also be attributed to the small distortion occurring in the ring fusion with equatorial hydroxy group. Further, the configuration of the hydroxy group in the α-forms of 2-aryl-*trans*-decahydroquinolin-4-ols **(1,3,5,7; Fig. 1**) was equatorial and that in β-forms **(2,4,6,8;** Fig.1) was axial. The same conclusion was also observed by Baliah and Natarajan.[24]

Introduction of *para*-substituent in phenyl ring (*p*-CH_3, **3**; *p*-OCH_3, **4**; **Fig. 1**) appeared to have no significant influence on the carbon chemical shifts in the decahydroquinoline system. But when *O*-Chloro substituent (**5, Fig.1**) was introduced in the phenyl ring, upfield shifts were observed for carbons 2 and 3. The chlorine substituent parameters were obtained by comparing the chemical shifts of 2-phenyl-*trans*-decahydroquinolin-4-ols with those of the corresponding 2-***0***-chlorophenyl-trans-decahydroquinolin-4-ols. Comparison of chemical shift data for **1** and **5** revealed that the O- -chloro group caused an upfield shift of C-2 and C-3. Thus in 5, the upfield shifts produced on C-2 and C-3 were found to be $\Delta\delta$ 4.5 and 1-8 ppm respectively. Similarly, upfield shifts produced for C-2 are C-3 in **6** were $\Delta\delta$ 3.2 and 2.0 ppm respectively. Probably the shielding of C-2 and C-3 might be attributed to the γ- and δ-shielding effect of 2'-Cl substituent.

^{13}C NMR spectral data of 3-methyl-2-phenyl-*trans*-decahydroquinolin-4-ols were given in **Table 7**. For calculation of the chemical shifts for carbon atoms in these compounds, 3,5-dimethyl-2,6-diaryl-piperidine, and its 4-hydroxy derivatives were taken as the reasonable model compounds. However, chemical shift values for these compounds were not available in literature and hence 2-phenyl-*trans*-decahydroquinolin-4-ols were chosen as models. The empirical substituent parameters for methyl group (already derived) were added to the chemical shifts of carbons in the said models to get the chemical shift values for compounds **9** to **16** and the values were reported in Table-7.

Table 7: ^{13}C Chemical shifts for 3-methyl-2-aryl-trans-decahydroquinolin-4-ols

No.	C2	C3	C4	C5	C6	C7	C8	C9	C10	Methyl	Aromatic Carbons
9.	67.2	45.3	79.6	27.9	25.7	25.0	33.2	59.7	49.7	14.5	127.4
											127.9
											128.4
											142.8
	(67.0)	(45.3)	(79.3)	(27.5)	(25.7)	(25.1)	(33.2)	(59.6)	(50.3)	---	
10	62.0	42.7	74.1	25.0	27.6	26.1	33.2	54.4	47.7	14.7	127.2
											127.9
											128.3
											143.4
	(61.0)	(43.9)	(72.0)	(24.7)	(27.3)	(25.8)	(33.4)	(54.1)	(46.3)	---	
11	66.8	45.2	79.5	27.9	25.6	25.0	33.1	59.6	49.6	14.5	127.8
											128.9
											136.9
											139.8
	(67.0)	(45.3)	(79.3)	(27.5)	(25.7)	(25.1)	33.20)	(59.6)	(50.3)	---	
12	61.6	42.6	74.1	25.0	27.7	26.2	33.6	54.4	47.7	14.8	127.8
											128.9
											136.8
											140.5

	(61.0)	(43.9)	(72.0)	(24.7)	(27.3)	(25.8)	(33.4)	(54.1)	(46.3)	---	
C.No.	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**	**C9**	**C10**	**Methyl**	**Aromatic Carbons**
13	67.1	45.3	79.5	27.8	25.6	24.9	33.1	59.6	49.6	14.5	127.4
											127.9
											128.3
											142.8
	(67.0)	(45.3)	(79.3)	(27.5)	(25.7)	(25.1)	(33.2)	(59.6)	(52.3)	---	
14	60.3	42.1	71.9	24.2	26.9	25.3	32.7	53.4	47.0	14.1	127.4
											131.4
											138.6
											141.7
	(61.0)	(43.9)	(72.0)	(24.7)	(27.3)	(25.8)	(33.4)	(54.1)	(46.3)	---	
15	66.5	45.1	49.6	27.9	25.7	25.0	33.1	59.6	49.6	14.5	113.7
											128.9
											135.1
											158.8
	(67.0)	(45.3)	(79.3)	(27.5)	(25.7)	(25.1)	(33.2)	(59.6)	(50.3)	---	
16	61.3	42.8	74.1	25.0	27.7	26.2	33.6	54.4	47.7	14.8	113.7
											128.8
											135.7
											158.7
	(61.0)	(43.9)	(72.0)	(24.7)	(27.3)	(25.8)	(33.4)	(54.1)	(46.3)	---	

The observed and calculated values were in good agreement with each, indicating the equatorial configuration of the methyl group in these compounds. The methyl carbon shift in 3-methyl-2-aryl-*trans*-decahydroquinolin-4-ols was found to be at 14.5 + 0.4 ppm. This value is very low when compared with methyl shift in methyl cyclohexanes (22.2 ppm). It was known that NH, hydroxyl, and phenyl groups have a shielding influence on the methyl shifts, and the total shielding effect of these groups might be considered to be approximately equal to $\Delta\delta$ 7.7 ppm. The chemical shift value for methyl group was found to be comparable to those obtained for 3-methyl-2,6-diarylpiperidine-4-ols, and 1,3-dimethyl-2,6-diarylpiperidine-4-ols[10].

Table 8: ^{13}C Chemical shifts for N-methyl-trans-decahydroquinolin-4-1ols

C.No.	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**	**C9**	**C10**	**C-CH_3/ N-CH_3**	**Aromatic Carbons**

18	64.0	43.3	67.6	25.3	28.7	25.6	30.6	61.5	45.5	---/	126.4
										39.2	127.3
											128.1
											145.6
	(65.4)	(41.1)	(67.7)	(25.0)	(27.0)	(25.9)	(29.8)	(61.5)	(4.83)	---/	

	(63.2)	(35.1)	(68.5)	(25.6)	(27.3)	(25.8)	(30.1)	(57.1)	(35.4)	---/	

19	78.4	44.9	75.9	28.4	25.3	25.2	30.7	66.8	48.2	15.3/	126.9
										39.7	128.3
											128.5
											143.2
	(78.0)	(43.8)	(79.7)	(28.2)	(25.4)	(25.1)	(29.6)	(67.1)	(48.3)	---/	

	(75.8)	(37.8)	(80.5)	(28.8)	(25.7)	(25.0)	(29.9)	(62.7)	(40.9)	---/	

20	73.8	42.2	70.5	25.5	28.9	25.9	31.1	61.3	46.1	15.9/	126.8
										39.6	128.1
											128.3
											143.7
	(72.8)	(41.2)	(74.2)	(25.3)	(27.3)	(26.2)	(29.6)	(61.8)	(46.3)	---/	

	(70.6)	(35.2)	(75.0)	(25.9)	(27.6)	(26.1)	(29.9)	(57.4)	(36.9)	---/	
										---	

*Values in parentheses are calculated values. Second line were those obtained by considering N-CH_3 equatorial. Third line were those obtained by considering N-CH_3 axial. Compound **17** could not be synthesized, hence spectra was not recorded.*

The ^{13}C NMR spectra of N-Methyl-2-phenyl-*trans*-decahydroquinolin-4-ol (β-form, **18**) and 1,3-dimethyl-2-phenyl-*trans*-decahydroquinolin-4-ols (α-and β-forms, **19** and **20**) were given in table-8. Assignment of the signal was made by comparing the signal positions with those of corresponding N-unsubstituted compounds, that is compounds **2,9,10,** and incorporating the N-CH_3 substituent parameters. The average values of N-CH_3 substituent parameters were taken from those reported by Eliel and Vierhapper[13] (**Table 9**).

Table 9: Effect of axial and equatorial N-CH_3 groups on ring carbon shifts in *trans*-decahydroquinoline

Ring Carbon	**Axial N-CH_3**	**Equatorial N-CH_3**
C_2	+8.6 ± 0.1	+10.8 ± 0.2
C_3	-7.5 ± 0.1	-1.5 ± 0.4
C_4	+0.9 ± 0.1	+0.1 ± 0.2
C_5	+0.9 ± 0.2	+0.3 ± 0.1
C_6	---	-0.3 ± 0.1
C_7	---	+0.1 ± 0.1
C_8	-3.3 ± 0.3	-3.6 ± 0.2
C_9	+3.0 ± 0.2	+7.4 ± 0.3
C_{10}	-10.8 ± 0.8	-1.4 ± 0.1

An examination of **Table 9**, revealed that the calculated values obtained by considering the N-CH_3 to be equatorial were in close agreement with the experimental values except for C-4 in 19 and 20. The upfield shift found in these compounds might be due to a slight distortion of the heterocyclic ring of the *trans*-decahydroquinoline system. Further, it might be concluded that N-CH_3 group in **18, 19,** and **20** had a preference for equatorial position.

The methyl group signal of N-CH_3 group was assigned at 39.2, 39.7, and 39.6 ppm in compounds **18, 19,** and **20** respectively. From the signal position, it might be concluded that the CH_3 group had greater preference for equatorial position. It is justified on the grounds that in decahydroquinoline systems the methyl signal of N-CH_3 group occurred at 42.5 + 0.6 ppm when the methyl group occupied an equatorial position[25, 26]. Considering the average shift of N-CH_3 signal from these compounds **18, 19,** and **20** at 39.5+0.4 ppm, an upfield shift of nearly $\Delta\delta$ 2.7 ppm might be due to the steric interaction of methyl and adjacent phenyl group in these compounds. In fact, such upfield shifts have been reported for methyl of N-CH_3 group when there was an equatorial substituent in 2-position in *trans*-decahydroquinoline system[13] as well as cyclohexane system[27]. Further, the absence of any signal at 33.2 ppm, which is due to an axial N-CH_3 group[25, 26, 28] was also in favour of the above conclusion that the methyl group on nitrogen had greater preference for an equatorial position. Similarly, the 13C NMR spectroscopy is helping to characterize the other fused ring systems like indoles[29].

Conclusion:

In this investigation, the authors succeeded in applying proton decoupled ^{13}C NMR spectroscopic technique for the study of conformations of differently substituted 2-aryl-*trans*-decahydroquinolin-4-ols. Based on comparative data between the experimental and calculated values the fusion of the rings in 2-aryl-*trans*-decahydroquinolin-4-ols was conclusively proved to be *trans-* from. An examination of the ^{13}C chemical shift values indicated that, the configuration of the hydroxyl group at C-4 was equatorial in all the α- forms of 2-aryl-*trans*-decahydroquinolin-4-ols and that of β- form's was axial. In 3-Methyl-2-aryl-*trans*-decahydroquinolin-4-ols the chemical shifts suggested equatorial configuration to methyl and phenyl groups. In case of 1-Methyl- and 1,3-dimethyl-2-aryl-*trans*-decahydroquinolin-4-ols the 1- or N-methyl group has a greater preference to the equatorial position.

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