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Comparative Study of Experimental and Theoretical Calculation on Synthesis of Substituted Indole by Gold(I)-Catalyst and DFT-STUDY based on ωb97xd/3-21g* Level for Fukui-Function and Chemical Shift of ^{1}H, ^{13}C NMR-Calculations †

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Abstract: The initial results on a novel procedure for the synthesis of benzo[*b*]carbazols *via* gold(I)-catalyzed tandem cyclization/Migration/cyclization is described. The procedure allowed the access to a highly functionalized benzo[*b*]carbazols in a one-pot process starting from tertiary anilines. The mechanism of this reaction by using gold(I) catalysis, interestingly proceeded via 5-*endo*-dig cyclization with successively migration of benzyl substituent on 2 and 3 position of indole, leading to the formation of benzyl substituted indole derivatives which is confirmed by ^{1}H, ^{13}C and NOE spectrum. Based on this experimental part of our initial results, we started DFT-study based on wb97xd/3-21g* level for fukui-function and chemical shift of ^{1}H, ^{13}C-NMR-calculations for Comparative study of Experimental and theoretical calculations.

Keywords: indole; gold(I)-catalyst; DFT; fukui function

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1. Introduction

Carbazole derivatives are known to have important photo physical and biological properties [1,2]. Carbazoles represent an important class of nitrogen containing heterocyclic compounds, many of which have found a wide range of applications as Natural product, Anticancer and biologically active agents in medicinal chemistry [3–5] (Figure 1).

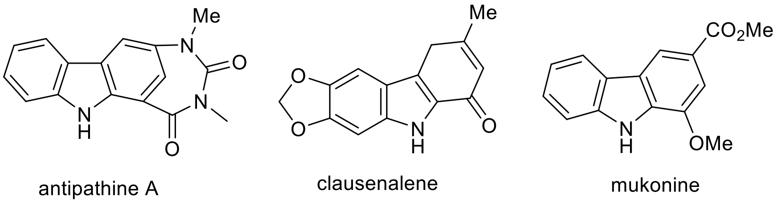


Figure 1. Natural product containing carbazole moiety.

Inspired from carbazole application and above discussion. We decide to Synthesis of Benzo(*b*)carbazols by tandem Au(I)-Catalyzed cyclization/migration/cyclization. Our aim to synthesized Benzo(*b*)carbazole with different substituents on that and make broad scope in this methodology.

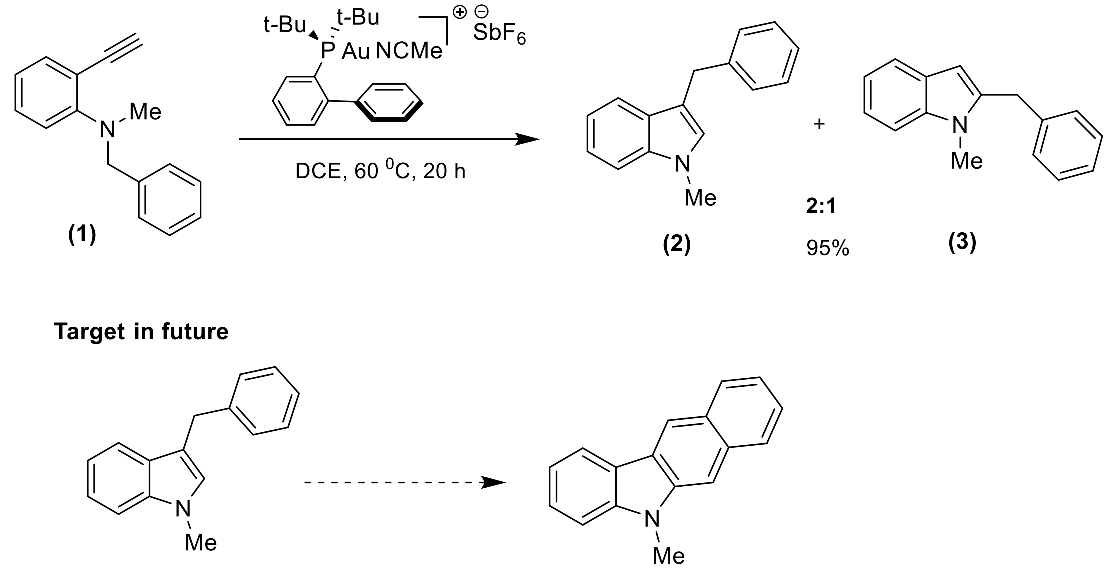
Besides the experimental part of our initial results, we started DFT-study based on ωb97xd/3-21g* level for fukui-function [6] and chemical shift of ^{1}H,^{13}C-NMR-calculations for Comparative study of Experimental and theoretical.

2. Results and Discussion

Results and discussion about both experimental and theoretical calculations is as started from bellow.

2.1. Experimental Results and Discussion

Gold-Catalyzed Reaction (Scheme 1):



Scheme 1. Gold(I)-catalyzed reaction.

The initial results on a novel procedure for the synthesis of benzo[*b*]carbazols via gold(I)-catalyzed tandem cyclization/Migration/cyclization is described. The procedure allowed the access to a highly functionalized benzo[*b*]carbazols in a one-pot process starting from tertiary anilines. The mechanism of this reaction by using gold(I) catalysis, interestingly proceeded via 5-*endo*-dig cyclization with successively migration of benzyl substituent on 2 and 3 position of indole, leading to the formation of benzyl substituted indole derivatives. We are proposing a cyclodimerization and aromatization via *6-exo-dig* with the help of gold(I)-carbene. Initial optimization with Tertiary Aniline 1, 5mol% of (Acetonitrile)[(2-biphenyl)di-*tert*-butylphosphine]gold(I) hexafluoroantimonate as Gold(I)-catalyst, Dry-DCM or Dry-DCE at 23 °C. But unfortunately, we do not get result. Then we rise the temp of reaction in Dry-DCE upto 60 °C with 10 mol% of gold(I) catalyst and then we get substituted indole 2 and 3 as a cyclized product with 95% yield which is confirmed by ^{1}H, ^{13}C and NOE spectrum.

2.2. Theoretical Results and Discussion

We started DFT-study based on ωb97xd/3-21g* level for fukui-functions and chemical shift of ^{1}H, ^{13}C NMR-calculation for Comparative study of Experimental and theoretical discussion is as shown in below.

A. Fukui-function calculation- for Tertiary-aniline

DFT-study based on ωb97xd/3-21g* level of fukui-functions calculation for tertiary-aniline **1**, to check the reactivity pattern and confirmation about cyclization by gold(I)-

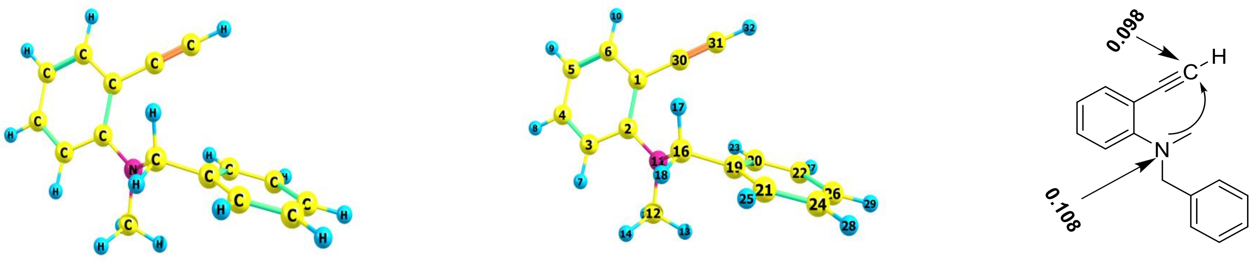
catalyst. In this fukui function calculation, we calculate the NBO-Charges and fukui-function value is as shown in bellow table-

According to Table 1 and Figure 2a–c and their results shows the fukui-functions value for the indications of reactivity pattern of tertiary-aniline **1**. this fukui-functions value gives the concrete proof and support to the cyclization with the formation five member N-containing ring was happened in tertiary aniline by gold(I)-catalyzed reaction. The tertiary-aniline fukui function value for all atom is in the Table 1. and selective fukui-function value for the indication of cyclization in tertiary aniline with the reactive site of nitrogen and terminal carbon of acetylene is as shown in Figure 2a–c.

Table 1. NBO-charges and fukui-function values calculations of tertiary-aniline.

Atom no.	Atom	NBO Charges (Neutral)	NBO Charges (Cation)	NBO Charges (Anion)	f+	f-	f0
1	C	-0.12523	-0.073112	-0.168685	0.052118	0.043455	0.0477865
2	C	0.346441	0.332116	0.302259	-0.014325	0.044182	0.0149285
3	C	-0.217884	-0.173519	-0.236299	0.044365	0.018415	0.03139
4	C	-0.21764	-0.204903	-0.282554	0.012737	0.064914	0.0388255
5	C	-0.224256	-0.181533	-0.229107	0.042723	0.004851	0.023787
6	C	-0.201176	-0.184691	-0.23982	0.016485	0.038644	0.0275645
7	H	0.21871	0.273837	0.141161	0.055127	0.077549	0.066338
8	H	0.221345	0.288591	0.119879	0.067246	0.101466	0.084356
9	H	0.219135	0.2955	0.135655	0.076365	0.08348	0.0799225
10	H	0.227837	0.287787	0.146173	0.05995	0.081664	0.070807
11	N	-0.717549	-0.609283	-0.7165	0.108266	-0.001049	0.0536085
12	C	-0.435301	-0.490949	-0.407384	-0.055648	-0.027917	-0.0417825
13	H	0.248291	0.316973	0.20527	0.068682	0.043021	0.0558515
14	H	0.194605	0.279206	0.160356	0.084601	0.034249	0.059425
15	H	0.230057	0.286122	0.211277	0.056065	0.01878	0.0374225
16	C	-0.267013	-0.313952	-0.251665	-0.046939	-0.015348	-0.0311435
17	H	0.272815	0.308842	0.283657	0.036027	-0.010842	0.0125925
18	H	0.210951	0.288666	0.168915	0.077715	0.042036	0.0598755
19	C	-0.012367	-0.022256	-0.007511	-0.009889	-0.004856	-0.0073725
20	C	-0.20411	-0.216027	-0.191797	-0.011917	-0.012313	-0.012115
21	C	-0.227376	-0.220226	-0.230569	0.00715	0.003193	0.0051715
22	C	-0.221705	-0.212066	-0.226507	0.009639	0.004802	0.0072205
23	H	0.239109	0.220374	0.258951	-0.018735	-0.019842	-0.0192885
24	C	-0.217275	-0.208623	-0.223365	0.008652	0.00609	0.007371
25	H	0.209438	0.232341	0.189733	0.022903	0.019705	0.021304
26	C	-0.222927	-0.212549	-0.231045	0.010378	0.008118	0.009248
27	H	0.217691	0.249021	0.19506	0.03133	0.022631	0.0269805
28	H	0.217058	0.254874	0.184605	0.037816	0.032453	0.0351345
29	H	0.216628	0.255576	0.183293	0.038948	0.033335	0.0361415
30	C	0.091315	0.070796	0.063919	-0.020519	0.027396	0.0034385
31	C	-0.366496	-0.268478	-0.516199	**0.098018**	**0.149703**	0.1238605
32	H	0.296876	0.351547	0.208842	0.054671	0.088034	0.0713525

f = fukui function.



(**a**) (**b**) (**c**)

Figure 2. Structures related to tertiary aniline (**a**) Structure of tertiary-aniline**.** (**b**) Structure of tertiary-aniline with numbering to the atom. (**c**) Structure of tertiary-aniline with fukui-function values.

B. Chemical-shift calculations of ^{1}H and ^{13}C-spectrum

The chemical-shift values calculations of ^{1}H and ^{13}C-spectrum of Tertiary-aniline **1** and Substituted-indole **2**, by DFT-study based on ωb97xd/3-21g* level for chemical shift of ^{1}H, ^{13}C NMR-calculations for comparative study of experimental and theoretical spectrum with their data.

a. Tertiary aniline chemical shift values of H^1, C^{13}-Spectrum calculations (Figure 3)

(i) (ii)

Figure 3. Structures related to Tertiary aniline. (**i**) structure of tertiary-aniline. (**ii**) Structure of aniline with numbering to the atom.

Table 2. ^{1}H-Chemical shift calculation of Tertiary aniline in Gas-phase and THF-Phase.

	TMS (GP)(IV)	TMS-THF (IV)	Hn	Aniline (GP)(IV)	Hn	Aniline-THF (IV)	Chemical-shift-Aniline (GP)	Chemical-shift-Aniline-THF
C-Atom	201.8241	202.7277	H-7	26.4314	H-7	26.027	6.3116	6.649
H-Atom	32.743	32.676	H-8	25.9201	H-8	25.5322	6.8229	7.1438
			H-9	26.3647	H-9	26.0451	6.3783	6.6309
			H-10	25.6915	H-10	25.4279	7.0515	7.2481
			H-13	30.0641	H-13	30.1041	2.6789	2.5719
			H-14	30.4061	H-14	30.1236	2.3369	2.5524
			H-15	30.3179	H-15	30.1474	2.4251	2.5286
			H-17	27.6159	H-17	27.6386	5.1271	5.0374
			H-18	29.3551	H-18	28.9913	3.3879	3.6847
			H-23	24.5794	H-23	24.5803	8.1636	8.0957
			H-25	25.9512	H-25	25.5687	6.7918	7.1073
			H-27	25.6609	H-27	25.3581	7.0821	7.3179
			H-28	25.7812	H-28	25.4341	6.9618	7.2419
			H-29	25.7587	H-29	25.4367	6.9843	7.2393
			H-32	29.7808	H-32	29.2971	2.9622	3.3789

TMS = Tetramethylsilane. GP = Gas Phase. THF = Tetrahydrofuran solvent Phase. Aniline = Tertiary aniline. Cn = Numbering to carbon atom in aniline. Hn = Numbering to hydrogen atom in aniline, δ = Chemical shift value.

Table 3. ^{13}C-Chemical shift calculation of Tertiary aniline in Gas-phase and THF-Phase.

	TMS (GP)(IV)	TMS-THF (IV)	Cn	Aniline (GP)(IV)	Cn	Aniline-THF (IV)	Chemical-shift Aniline (GP)	Chemical-shift-Aniline-THF
C-Atom	201.8241	202.7277	C-1	104.3368	C-1	105.7009	97.4873	97.0268
H-Atom	32.743	32.676	C-2	68.0364	C-2	67.4919	133.7877	135.2358
			C-3	101.2636	C-3	100.5492	100.5605	102.1785
			C-4	90.5995	C-4	89.4183	111.2246	113.3094
			C-5	99.9484	C-5	99.9144	101.8757	102.8133
			C-6	85.0725	C-6	85.1051	116.7516	117.6226
			C-12	173.032	C-12	173.3516	28.7921	29.3761
			C-16	152.104	C-16	152.4743	49.7201	50.2534
			C-19	80.628	C-19	79.474	121.1961	123.2537
			C-20	90.3088	C-20	90.734	111.5153	111.9937
			C-21	92.3104	C-21	91.8087	109.5137	110.919
			C-22	91.895	C-22	91.7152	109.9291	111.0125
			C-24	92.3706	C-24	91.6962	109.4535	111.0315
			C-26	92.8633	C-26	92.6526	108.9608	110.0751
			C-30	133.5442	C-30	132.9856	68.2799	69.7421
			C-31	126.7677	C-31	126.3533	75.0564	76.3744

TMS = Tetramethylsilane. GP = Gas Phase. THF = Tetrahydrofuran Solvent Phase. Aniline = Tertiary aniline. Cn = Numbering to carbon atom in aniline. Hn = Numbering to hydrogen atom in aniline, δ = Chemical shift value.

2.2.1. Experimental Data of Tertiary aniline

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.81 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.29 – 7.16 (m, 4H), 7.03 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.73 (td, *J* = 7.5, 1.5 Hz, 1H), 4.05 (s, 2H), 2.55 (s, 3H), 1.48 (s, 1H).

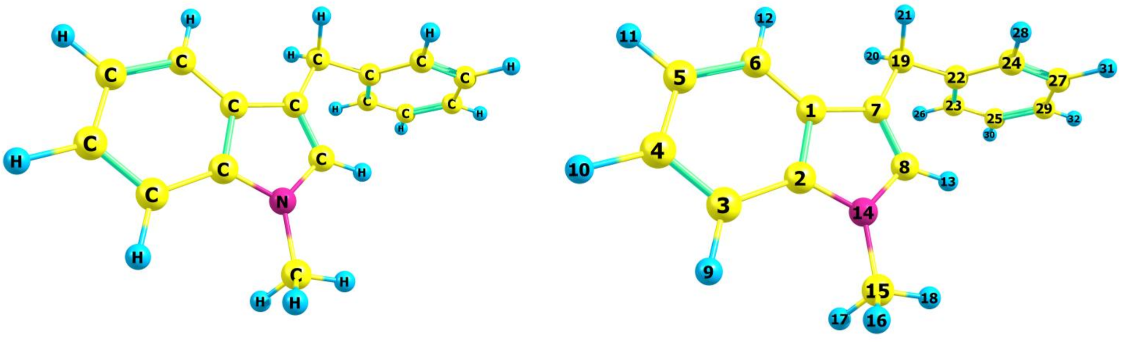
^{13}C NMR (126 MHz, Chloroform-*d*) δ 154.25, 140.26, 138.35, 129.16, 128.86, 128.35, 127.25, 125.62, 122.43, 98.70, 61.27, 41.73.

Table 4. Tertiary aniline comparative δ-value with experimental and calculated (Gas-phase and THF-solvent Phase) ^{1}H, ^{13}C-spectra.

Cn	Exp. δ–value	Aniline GP-δ–value	Aniline THF-δ–value	Hn	Exp. δ–value	Aniline GP-δ–value	Aniline THF-δ–value
C-1	140	97.4873	97.0268	H-7	7.3	6.3	6.649
C-2	154	133.7877	135.2358	H-8	7.4-7.3	6.8229	7.1438
C-3	128.3	100.5605	102.1785	H-9	7.4-7.3	6.3783	6.6309
C-4	129	111.2246	113.3094	H-10	7.81	7.0515	7.2481
C-5	128.8	101.8757	102.8133	H-13	2.55	2.6789	2.5719
C-6	128	116.7516	117.6226	H-14	2.55	2.3369	2.5524
C-12	41	28.7921	29.3761	H-15	2.55	2.4251	2.5286
C-16	61	49.7201	50.2534	H-17	4.2	5.1271	5.0374
C-19	138	121.1961	123.2537	H-18	4.2	3.3879	3.6847
C-20	127	111.5153	111.9937	H-23	7.29-7.16	8.1636	8.0957
C-21	127	109.5137	110.919	H-25	6.73	6.7918	7.1073
C-22	127	109.9291	111.0125	H-27	7.29-7.16	7.0821	7.3179
C-24	127	109.4535	111.0315	H-28	7.29-7.16	6.9618	7.2419
C-26	122	108.9608	110.0751	H-29	7.29-7.16	6.9843	7.2393
C-30	125	68.2799	69.7421	H-32	1.48	2.9622	3.3789
C-31	98	75.0564	76.3744				

TMS = Tetramethylsilane. GP = Gas Phase. THF = Tetrahydrofuran solvent phase. Aniline = Tertiary aniline. Cn = Numbering to carbon atom in aniline. Hn = Numbering to hydrogen atom in aniline. Exp = Experimental Chemical shift value. δ = Chemical shift value.

b. Substituted-indole chemical shift values of ^{1}H, ^{13}C-Spectrum calculations (Figure 4)



(i) (ii)

Figure 4. Structures related to Substituted indole. (**i**) structure of Substituted-indole. (**ii**) Structure of Substituted-indole with numbering to the atom.

Table 5. ^{1}H-Chemical shift calculation of 3-Benzyl-1-methyl-1*H*-indole in Gas-phase and THF-Phase.

	TMS (GP)(IV)	TMS-THF (IV)	Hn	Indole (GP)(IV)	Hn	Indole-THF (IV)	Chemical-shift-indole (GP)	Chemical-shift-indole-THF
C-Atom	201.8241	202.7277	H-9	26.2236	H-9	25.7561	6.5194	6.9199
H-Atom	32.743	32.676	H-10	25.9035	H-10	25.5998	6.8395	7.0762
			H-11	25.9964	H-11	25.725	6.7466	6.951
			H-12	25.6208	H-12	25.294	7.1222	7.382
			H-13	27.666	H-13	27.3179	5.077	5.3581
			H-16	29.3468	H-16	29.1403	3.3962	3.5357
			H-17	29.3468	H-17	29.1403	3.3962	3.5357
			H-18	29.6463	H-18	29.2479	3.0967	3.4281
			H-20	29.1511	H-20	28.9568	3.5919	3.7192
			H-21	29.1511	H-21	28.9568	3.5919	3.7192
			H-26	25.7098	H-26	25.4248	7.0332	7.2512
			H-28	25.7098	H-28	25.4248	7.0332	7.2512
			H-30	25.7424	H-30	25.4082	7.0006	7.2678
			H-31	25.7424	H-31	25.4082	7.0006	7.2678
			H-32	25.8053	H-32	25.4725	6.9377	7.2035

TMS = Tetramethylsilane. GP = Gas Phase. THF = Tetrahydrofuran solvent phase. Indole = 3-Benzyl-1-methyl-1*H*-indole Cn = Numbering to carbon atom in Indole. Hn = Numbering to hydrogen atom in Indole. Exp = Experimental Chemical shift value. δ = Chemical shift value.

Table 6. ^{13}C-Chemical shift calculation of 3-Benzyl-1-methyl-1*H*-indole in Gas-phase and THF-Phase.

	TMS (GP)(IV)	TMS-THF (IV)	Cn	Indole (GP)(IV)	Cn	Indole-THF (IV)	Chemical-shift Indole (GP)	Chemical-shift-Indole-THF
C-Atom	201.8241	202.7277	C-1	91.9216	C-1	92.9679	109.9025	109.7598
H-Atom	32.743	32.676	C-2	85.3562	C-2	85.4278	116.4679	117.2999
			C-3	108.7586	C-3	107.6856	93.0655	95.0421
			C-4	97.0911	C-4	97.1603	104.733	105.5674
			C-5	99.4799	C-5	99.8223	102.3442	102.9054
			C-6	99.0845	C-6	99.0496	102.7396	103.6781
			C-7	100.5131	C-7	101.0417	101.311	101.686
			C-8	89.861	C-8	88.9286	111.9631	113.7991
			C-15	175.9563	C-15	176.269	25.8678	26.4587
			C-19	175.1324	C-19	175.9396	26.6917	26.7881
			C-22	80.3038	C-22	79.6592	121.5203	123.0685
			C-23	89.8969	C-23	89.6599	111.9272	113.0678
			C-24	89.8969	C-24	89.6599	111.9272	113.0678
			C-25	91.7282	C-25	91.2224	110.0959	111.5053
			C-27	91.7282	C-27	91.2224	110.0959	111.5053
			C-29	93.737	C-29	93.29	108.0871	109.4377

TMS = Tetramethylsilane. GP = Gas Phase. THF= Tetrahydrofuran solvent phase. Indole = 3-Benzyl-1-methyl-1*H*-indole Cn = Numbering to carbon atom in Indole. Hn=Numbering to hydrogen atom in Indole. Exp = Experimental Chemical shift value. δ = Chemical shift value.

2.2.2. Experimental Data of 3-Benzyl-1-methyl-1H-indole

^{1}**H NMR** (300 MHz, $CDCl_3$) δ 7.63 (d, *J*) 7.9 Hz, 1H), 7.45-7.24 (m, 7H), 7.18 (m, 1H), 6.83 (s, 1H), 4.21 (s, 2H), 3.79 (s, 3H).

^{13}**C NMR** (75 MHz, CDCl3) δ 141.4, 137.1, 128.6, 128.3, 127.8, 127.1, 125.8, 121.5, 119.2, 118.7, 114.3, 109.1, 32.5, 31.5.

Table 7. 3-Benzyl-1-methyl-1*H*-indole comparative δ-value with experimental and calculated (Gas-phase and THF-solvent Phase) ^{1}H, ^{13}C-spectra.

Cn	Exp. δ-value	indole GP-δ-value	indole THF-δ-value	Hn	Exp. δ-value	indole GP-δ-value	indole THF-δ-value
C-1	128.6	109.9025	109.7598	H-9	7.63	6.5194	6.9199
C-2	141.4	116.4679	117.2999	H-10	7.45-7.24	6.8395	7.0762
C-3	127.8	93.0655	95.0421	H-11	7.45-7.24	6.7466	6.951
C-4	129	104.733	105.5674	H-12	7.18	7.1222	7.382
C-5	128.8	102.3442	102.9054	H-13	6.83	5.077	5.3581
C-6	128	102.7396	103.6781	H-16	3.79	3.3962	3.5357
C-7	128.3	101.311	101.686	H-17	3.79	3.3962	3.5357
C-8	137.1	111.9631	113.7991	H-18	3.79	3.0967	3.4218
C-15	31.5	25.8678	26.4587	H-20	4.21	3.5917	3.7192
C-19	32.5	26.6917	26.7881	H-21	4.21	3.5919	3.7192
C-22	118.7	121.5203	123.0685	H-26	7.45-7.24	7.0332	7.2512
C-23	119.2	111.9272	113.0678	H-28	7.45-7.24	7.0332	7.2512
C-24	119.2	111.9272	113.0678	H-30	7.45-7.24	7.0006	7.2678
C-25	119.2	110.0959	111.5053	H-31	7.45-7.24	7.0006	7.2678
C-27	119.2	110.0959	111.5053	H-32	7.45-7.24	6.9377	7.2035
C-29	109.1	108.0871	109.4377				

TMS = Tetramethylsilane. GP = Gas Phase. THF = Tetrahydrofuran solvent phase. Indole = 3-Benzyl-1-methyl-1*H*-indole Cn = Numbering to carbon atom in Indole. Hn = Numbering to hydrogen atom in Indole. Exp = Experimental Chemical shift value. δ = Chemical shift value.

According to the above results and discussion fukui-function calculation support the cyclization reaction and ^{1}H, ^{13}C NMR calculation shows diferent results than experimental.

3. Conclusions

(i). Bis alkylation on 2-iodo aniline with two different substituted benzyl moiety is difficult.
(ii). Migratory aptitude of benzyl group is more as compared to methyl group.
(iii). Cyclization and migration were happen in same reaction and condition.
(iv). We get first intermolecular cyclized product of benzyl substituted indole with excellent yield.
(v). Fukui-function calculations also support the reactivity and cyclization was happened in experimentally.
(vi). **^{1}H** and **^{13}C** chemical shift calculation shows the slightly difference chemical shift value than experimental based on ωb97xd/3-21g* Level.
(vii). We need to try ^{1}H and ^{13}C chemical shift calculation based on higher level of basis set.

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