

## ORIGINAL ARTICLE

## NMR spectra of Azobenzene-bridged calix [8] arene complexes by ab initio hartree-fock calculations as nanostructure compound

Masoumeh Sayadian <sup>1</sup>; Hamidreza Sadegh <sup>2, \*</sup>; Gomaa Abdelgawad Mohammed Ali <sup>3, 4</sup>

<sup>1</sup>Department of Chemistry, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran

<sup>2</sup>West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology and Engineering, Division of Functional Materials and Biomaterials, Al. Piastow 45, Szczecin, Poland

<sup>3</sup>Chemistry Department, Faculty of Science, Al-Azhar University, Assiut, 71524, Egypt

<sup>4</sup>Faculty of Industrial Sciences and Technology, University Malaysia Pahang, Gambang, 26300 Kuantan, Malaysia

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### Abstract

Calix[8]arenes of conformational rigid were isolated. The NMR parameters of the structure of calix[8]arenes have been compared. The study of organic structures to form nanoporous materials is well-known in chemistry phenomena to find the crystal form of calix[8]arene as supramolecule. Investigated and compared hydrogen bonding, oxygen and nitrogen atoms effect on calix[8]arene and its complexes were reported at Hartree-Fock (HF) theory by Gaussian 2003 of program package. In this work, the complexing properties of azobenzene-bridged calix[8]arene with alkali earth metal cations has studied. The complexation properties of calix[8]arene were studied by HF method. The complex of the calixarenes showed different properties for the different cations, depending on the cations and the position of the substituent grafted on the ligand.

**Keywords:** Calix [8] Arene; Chemical Shift; Density Functional Theory; Hartree-Fock; Hydrogen Bonding; Nanostructure

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## INTRODUCTION

In the recent years, the calixarenes are of particular interest as metal ion receptors [1-4]. The use of calix[n]arenes in analytical chemistry and separation chemical technology has been discussed [5]. It was founded that the cavity size, the position and kind of donor groups and the molecular flexibility have a pronounced impact on the complexation properties as well as the extraction power and selectivity [6, 7]. Calix[n]arenes have generated considerable interest due to their basket-shaped structure and as useful building blocks to synthesize selective receptors for the guest species, notably alkali, alkaline earth and transition metal cations [8, 9]. Supramolecular interaction is the vital initial process triggering biological and chemical events. Studies on binding between converging sites of synthetic hosts with

diverging sites of guest molecules, atoms or ions have progressively provided valuable information towards an understanding of the supermolecular interaction of complicated natural elements [10-12]. Much attention has recently been paid to achieve the binding selectivity between the host and the guest atoms by controlling the size and shape of the binding cleft of the host molecule [13]. A host molecule that can controllably switch its binding selectivity as desired is rare [14] but extremely desirable for various applications including imitating biological events. Owing to its pre-organized structure, calix[8]arene is one of the most established molecular platforms for constructing three-dimensional hosts for atoms or ions [15]. The structure of calix[8]arene consists of eight phenol rings linked together with four methylene units in a circular manner producing

\* Corresponding Author Email: [Hamid-sadegh@zut.edu.pl](mailto:Hamid-sadegh@zut.edu.pl)

a basket like architecture [16]. A high number of calculations have recently reported in the literature concerning the determination of NMR chemical shift (c.s.) by quantum chemistry methods [17-22]. Moreover, it is known that the density functional theory (DFT) method [23-25] takes into account electron correlation contributions, which are especially important in systems contained extensive electron conjugation and/or electron lone pairs [21]. Recently, DFT has been accepted by the quantum chemistry community as a cost-effective approach for the computation of molecular structure, vibration frequencies, and energies of chemical reactions. Many studies have shown that molecular structures and vibration frequencies calculated by DFT methods are more trustable than MP2 methods [26, 27]. While there is sufficient evidence that DFT provides an accurate description of the electronic and structural properties of interfaces and small molecules, relatively little is known about the symmetric performance of DFT applications to molecular associates. To further access the reliability of DFT methods applied to this field of chemistry, in this paper, the structure and bonding of the calix[8]arene as obtained by high-level ab initio calculations will be discussed. The role of basis set size and basis set superposition effects will be analyzed in detail. In the present study, we will perform a high-level of calculations and systematic analysis of the theoretical result will be obtained [28, 29].

## EXPERIMENTAL

### Computational section

The geometry optimization of the azobenzene-bridged calix[8]arene has been carried out using the GAUSSIAN 2003 programs package [29, 30]. The computational model consists of Geometries for calix[8]arene were fully optimized by Restricted Hartree-Fock (RHF) with STO-3G, 3-21G and 6-31G levels [30]. In this study, the NMR parameters of the title compound in the ground state have been calculated to compare with the experimental geometric parameters using the HF method. These calculations are valuable for providing insight into molecular parameters and NMR spectrum. To confirm the superiority of the DFT methods, HF method at the STO-3G, 3-21G and 6-31G basis set along with analytic NMR shielding tensors calculations were simultaneously adopted [30].

## RESULTS AND DISCUSSION

This study deals with azobenzene-bridged calix[8]arene molecule as a nanostructure compound for complexed by alkali or earth alkali cations. Before and after connecting the metal ions to calix[8]arene NMR calculations were performed in the electric field of charges. NMR parameters are listed in Table 1 in different levels and different basis sets.  $\sigma_{iso}$  (isotropic chemical shift) and  $\delta$  (chemical shift) curves versus atomic charges for calix[8]arene and calix[8] arene/alkali or earth alkali cations. These curves are drawn for different levels and different basic sets. Generally, all curves are similar. To assess the quality of the theoretical data, geometrical parameters available for calix[8]arene. In the compound, the C-H stretch is decreasing total charge, which indicates the increasing acidity of the CH hydrogen from CH-N to CH-O. This phenomenon may be attributed to the induced effect of the electronegative element. In addition, the charge distribution in this compound is of primary importance from the point of view of the CH-Y. One stable structure of the azobenzene-bridged calix[8]arene is shown in Fig. 1a, in addition, the structure with a metal ion is shown in Fig. 1b. Taking the calculated result of the seven complexes compared together.

As shown in Fig. 2a the most of the negative charges are attached to oxygen atoms and then it attached to nitrogen atoms. Similarly, the most of the positive charges are attached to hydrogen atoms that linked to oxygen atoms and then it attached to carbon atoms that linked to C-O bond. Initially, molecular structures of the title compound and  $^{13}\text{C}$  NMR,  $^1\text{H}$  and  $^{14}\text{N}$  calculations have been made by HF method. These results are shown in Table 1. As it is elaborated in Fig. 2b the most of the chemical shift attached to nitrogen atoms; for find reason notice to Fig. 1a although compound conjugated bonds must be aromatic theoretically but the aromaticity becomes not stable because of the spherical prohibition so that the configuration charges and the resonance occur between non-planar sheets; hence the chemical shift on the nitrogen atoms are under such more strong electrostatic field. As shown in Table 1 and Fig. 2c the least  $\sigma_{iso}$  is related to nitrogen atoms; that is because of conjugated bonds and aromaticity of the nitrogen bonds configuration and the resonance occur between non-planar sheets; hence the  $\sigma_{iso}$  on the nitrogen atoms is lower than another atom.

Table 1: Total charge, chemical shift and isotropic chemical shift of calix [8] arene at HF level.

No. Atom	Total charge (C)			$\delta$ (ppm)			$\sigma_{\text{iso}}$ (ppm)		
	6-31G	3-21G	STO-3G	6-31G	3-21G	STO-3G	6-31G	3-21G	STO-3G
27C	0.3037	0.3356	0.08883	83.33	71.789	79.092	52.473	71.774	106.015
47 C	0.2892	0.3344	0.09025	80.658	70.695	78.357	53.057	71.024	105.774
87 O	-0.8045	-0.7359	-0.2859	40.748	54.864	45.379	273.045	300.61	315.767
88 O	-0.8143	-0.7624	-0.2875	56.413	58.144	46.368	277.407	286.95	313.298
89 O	-0.8305	-0.7202	-0.2579	54.744	42.508	52.723	279.567	300.60	367.238
90 O	-0.8649	-0.8144	-0.3344	43.115	41.257	57.306	272.099	290.82	325.254
91 O	-0.8799	-0.7853	-0.2972	38.391	37.834	31.484	273.657	296.36	328.849
92 O	-0.8604	-0.5666	-0.3366	54.745	53.759	61.102	266.179	286.83	319.019
93 O	-0.8549	-0.8039	-0.3326	44.581	43.656	58.033	265.216	277.99	323.777
96 O	-0.8315	-0.7256	-0.2599	42.857	43.576	46.147	275.526	303.39	364.476
99 C	0.14946	0.2366	0.06948	111.688	99.807	99.089	52.742	70.465	104.294
105 C	0.16955	0.2423	0.0705	111.287	99.363	97.961	53.962	71.599	105.753
111 N	-0.3539	-0.3856	-0.1247	623.892	581.172	520.541	-408.31	-357.68	-264.65
112 N	-0.3358	-0.3771	-0.1227	616.789	574.407	514.298	-397.77	-348.11	-259.63
212 H	0.4368	0.4289	0.2031	10.917	14.758	10.521	31.691	31.373	31.419
213 H	0.5089	0.4547	0.2405	19.685	19.655	18.531	25.829	25.539	25.818
214 H	0.4451	0.4215	0.2202	10.263	11.018	8.501	29.624	29.859	29.266
215 H	0.4979	0.4415	0.2399	19.392	20.351	17.5	25.777	25.655	25.394
216 H	0.5094	0.4604	0.2364	15.299	16.633	15.231	27.825	26.359	26.965
217 H	0.2093	0.2522	0.0688	3.222	3.558	4.785	29.284	29.541	29.552
Dipole moment (Deby)				6-31G	3-21G	STO-3G			
				5.2938	4.3863	3.787			
Energy (kcal/mol)				-4639.63	-4615.71	-4584.88			

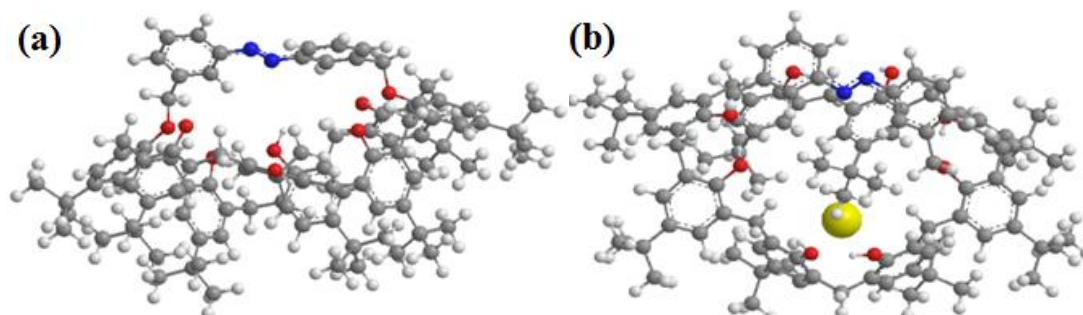


Fig. 1: The final optimization form of azobenzene-bridged calix [8] arene (a) and complexes with metal ion.

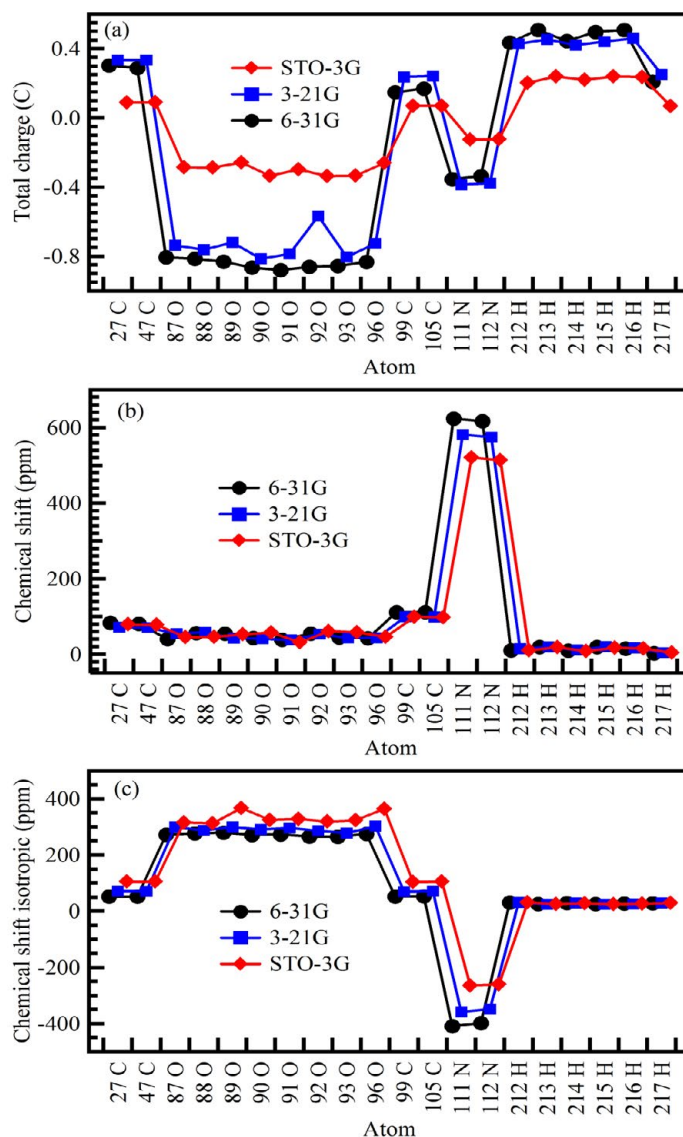


Fig. 2: Total charge (a), chemical shift (b) and chemical shift isotropic (c) vs. atom number of calix [8] arene.

As a notice, to Fig. 3a the total charge computed for Li-calix is higher than of Na-calix and K-calix complexes. That is due to the nuclear effective charge which is decreased from Li to K atom. For more detailed analysis, the role of metal ions effects, Table 2 gives a detailed analysis of the chemical shifts obtained with metal ions. NMR parameters calculation using ab initio techniques has become a major and powerful tool in the investigation of variation in the molecular structure.

The ability to quickly evaluate and correlate the magnitude and orientation of the chemical

shielding anisotropy tensor with variations in bond length, bond angles and local coordination and nearest neighbor interactions has seen in a high number of recent applications in the investigation of molecular structure. The chemical shifts of calix[8]arene atoms principal values in the available method were obtained. Moreover, diffuse and polarizable functions effects in basis sets are investigated on NMR shielding tensors. As expected, the chemical shift computed for Li-calix is higher than of Na-calix then K-calix complexes as shown in Figs. 3b and 3c. As shown in Fig. 3, all parameters computed for Li-calix is higher than of

Na-calix then K-calix complex.

In addition, shown in Table 3 for Ba-calix, Mg-calix and Ca-calix complexes, total charge, chemical shift and  $\sigma_{iso}$  computed for Ba-calix are higher than of Mg-calix then Ca-calix complex. In addition, the data were displayed in Figs. 4a, 4b and 4c. On the other hand, as shown in Table 4 and Figs. 5a, 5b and 5c, the study of Li-calix, Be-calix and B-calix complexes indicated total charge;

chemical shift and  $\sigma_{iso}$  computed for Li-calix are higher than of Be-calix then B-calix complexes. As it is elaborated in Table 5, the least of the energy is attached to Li-calix complex. This complex is the most stable among the other complexes as shown in Fig. 6a. The most dipole moment is related to Li-calix complex (see Fig. 6b) that is because of nuclear effective charge which is decreased from Li to B atoms.

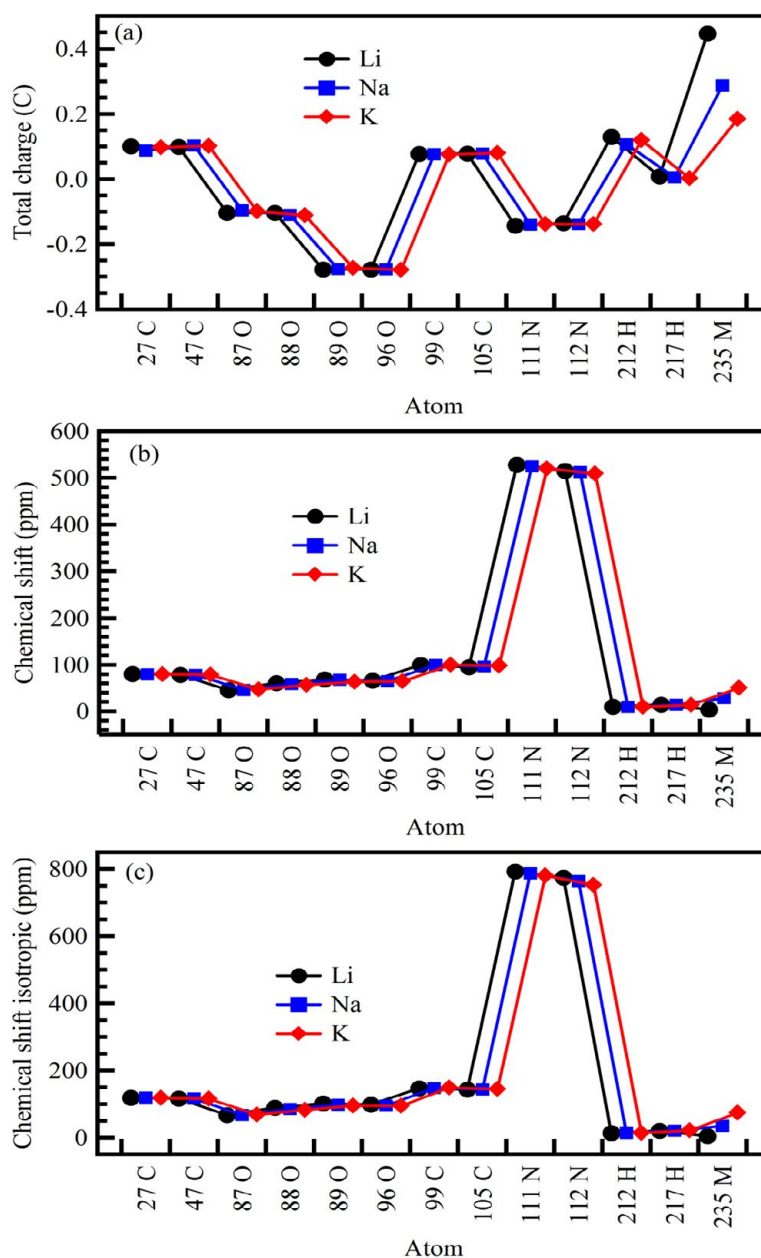


Fig. 3: Total charge (a), chemical shift (b) and chemical shift isotropic (c) vs. atom number of calix [8] arene with some alkali-earth metals.

Table 2: Total charge, chemical shift and isotropic chemical shift of calix [8] aren alkali earth metal complexes at HF level.

No. Atom	Total charge (C)			$\delta$ (ppm)			$\sigma_{iso}$ (ppm)		
	Li	Na	K	Li	Na	K	Li	Na	K
27 C	0.1012	0.0878	0.098	80.321	80.012	79.453	119.8753	119.1326	118.3672
47 C	0.0996	0.1035	0.102192	78.396	78.482	78.692	117.2165	116.9835	116.3581
87 O	-0.1035	-0.0957	-0.09866	45.385	45.998	46.779	67.4392	67.8193	68.6351
88 O	-0.1032	-0.1096	-0.11122	60.644	59.231	56.83	89.6799	85.2328	82.7964
89 O	-0.2770	-0.2763	-0.27247	68.705	68.431	63.121	102.3687	98.0054	95.3418
96 O	-0.2768	-0.2767	-0.27903	66.384	65.131	64.417	99.4352	95.6361	94.6076
99 C	0.0772	0.0763	0.075503	99.741	99.856	100.12	147.823	148.30485	149.3515
105 C	0.0784	0.0787	0.079742	95.021	96.459	97.805	143.8852	144.3817	145.1971
111 N	-0.1422	-0.1401	-0.13845	528.01	525.15	520.11	793.4193	787.7103	780.1554
112 N	-0.1346	-0.1383	-0.13778	515.44	512.87	509.19	774.3084	763.9931	752.5479
212 H	0.1297	0.1072	0.11925	10.155	9.8936	9.5643	14.5044	14.2805	14.0554
217 H	0.0087	0.0062	0.00238	14.486	14.256	14.153	20.8756	21.3912	21.643
235 M	0.4466	0.2876	0.18451	4.3581	28.295	50.246	5.361	35.1833	74.7442

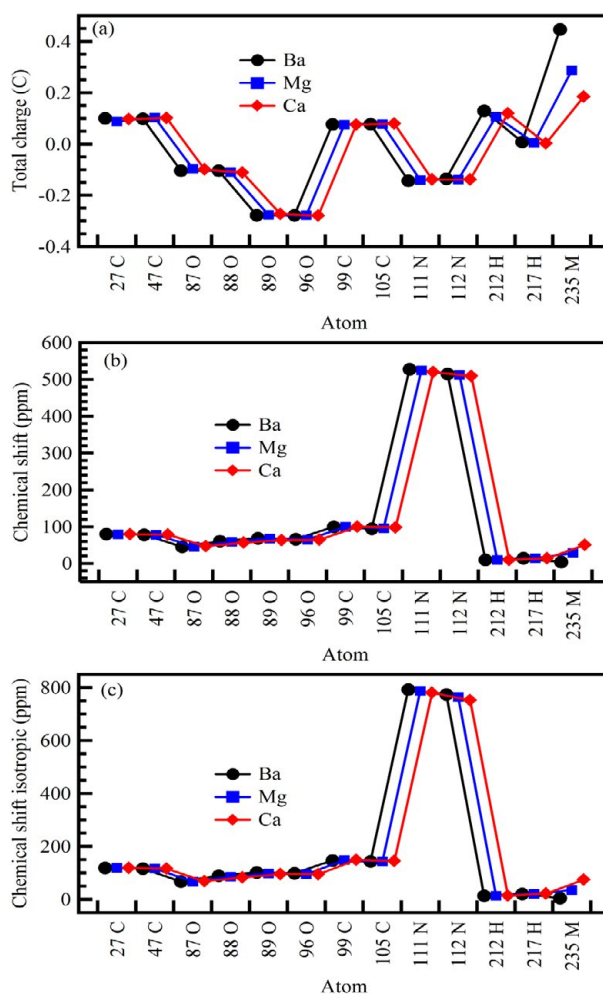


Fig. 4: Total charge (a), chemical shift (b) and chemical shift isotropic (c) vs. atom number of calix [8] arene with some alkali metals.

Table 3: Total charge, chemical shift and isotropic chemical shift of calix [8] aren alkali metal complexes at HF level.

No. Atom	Total charge (C)			$\delta$ (ppm)			$\sigma_{iso}$ (ppm)		
	Be	Mg	Ca	Be	Mg	Ca	Be	Mg	Ca
27 C	0.1015	0.1022	0.0993	80.002	79.632	79.231	107.51	107.492	107.445
47 C	0.0995	0.0998	0.0978	77.532	77.563	77.763	107.92	107.620	107.047
87 O	-0.108	-0.321	-0.4002	43.142	43.466	43.963	331.04	330.001	328.371
88 O	-0.103	-0.325	-0.4074	60.095	60.113	60.252	338.60	337.569	336.864
89 O	-0.277	-0.277	-0.4794	70.541	71.604	71.832	365.58	369.045	372.604
96 O	-0.276	-0.275	-0.4532	63.087	63.363	63.673	358.91	360.612	362.022
99 C	0.0768	0.0768	0.0755	97.768	97.030	97.659	111.85	110.432	109.884
105 C	0.0791	0.0792	0.0788	95.325	95.144	94.923	113.11	112.743	111.144
111 N	-0.142	-0.142	-0.1406	526.73	526.16	525.86	-244.3	-242.12	-240.460
112 N	-0.139	-0.138	-0.1434	519.10	519.43	518.54	-238.5	-226.34	-218.641
212 H	0.1322	0.1076	0.1006	10.208	8.576	7.994	31.22	31.9801	32.4908
217 H	0.0090	0.006	0.0058	14.431	16.106	16.121	29.617	28.0112	26.741
235 M	0.3782	0.2479	0.1107	14.510	57.779	84.217	144.21	115.250	95.2006

Table 4: Total charge, chemical shift and isotropic chemical shift of calix [8] aren IA, IIA and IIIA metal complexes at HF. level.

No. Atom	Total charge (C)			$\delta$ (ppm)			$\sigma_{iso}$ (ppm)		
	Li	Be	B	Li	Be	B	Li	Be	B
27 C	0.101	0.087	0.098	80.32	80.012	79.45	119.8	119.1	118.3
47 C	0.099	0.103	0.102	78.39	78.482	78.69	117.2	116.9	116.3
87 O	-0.10	-0.09	-0.09	45.38	45.998	46.77	67.43	67.81	68.63
88 O	-0.10	-0.10	-0.11	60.64	59.231	56.83	89.67	85.23	82.79
89 O	-0.27	-0.27	-0.27	68.70	68.431	63.12	102.3	98.00	95.34
96 O	-0.27	-0.27	-0.27	66.38	65.131	64.41	99.43	95.63	94.60
99 C	0.077	0.076	0.075	99.74	99.856	100.1	147.8	148.3	149.3
105 C	0.078	0.078	0.079	95.02	96.459	97.80	143.8	144.3	145.1
111 N	-0.14	-0.11	-0.13	528.0	525.15	520.1	793.4	787.7	780.1
112 N	-0.13	-0.13	-0.13	515.4	512.87	509.1	774.3	763.9	752.5
212 H	0.129	0.107	0.119	10.15	9.8936	9.56	14.50	14.28	14.05
217 H	0.008	0.006	0.002	14.48	14.256	14.15	20.87	21.39	21.64
235 M	0.446	0.287	0.184	4.358	28.295	50.24	5.361	35.18	74.74

Table 5: Energy and Dipole moment of calix [8] aren complexes at HF level.

Complex	Energy (Hartry)	Dipole moment (Deby)
Li-Calix	-4620.49	7.0503
Na-Calix	-4615.47	6.0173
K-Calix	-4608.03	5.8878
Be-Calix	-4612.47	5.7627
Mg-Calix	-4604.33	5.3296
Ca-Calix	-4595.25	5.3166
B-Calix	-4598.34	4.5324

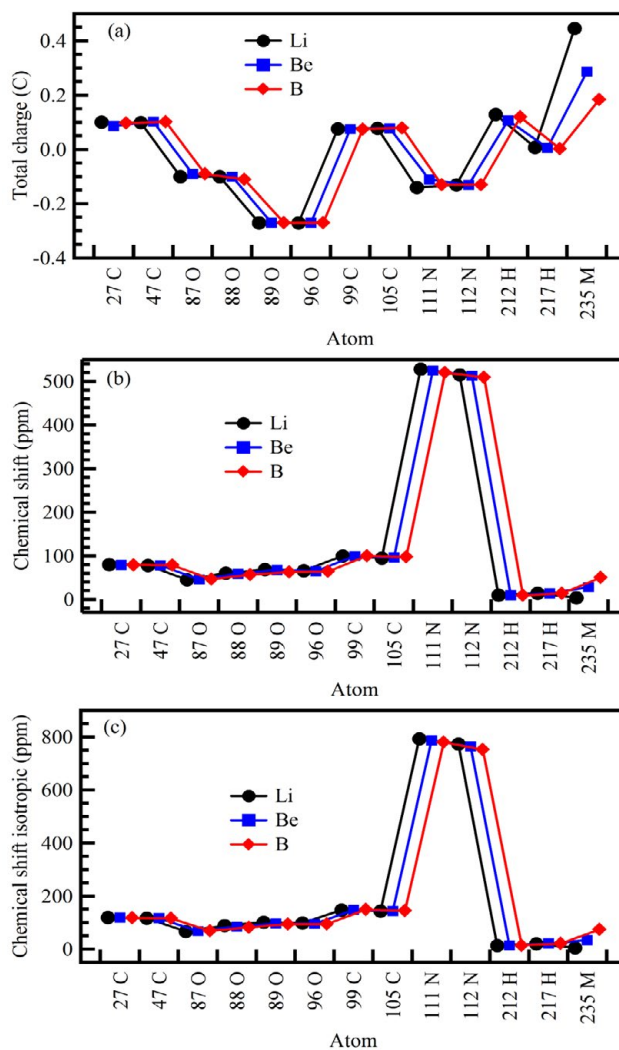


Fig. 5: Total charge (a), chemical shift (b) and chemical shift isotropic (c) vs. atom number of calix [8] arene with some IA, IIA and IIIA metals.

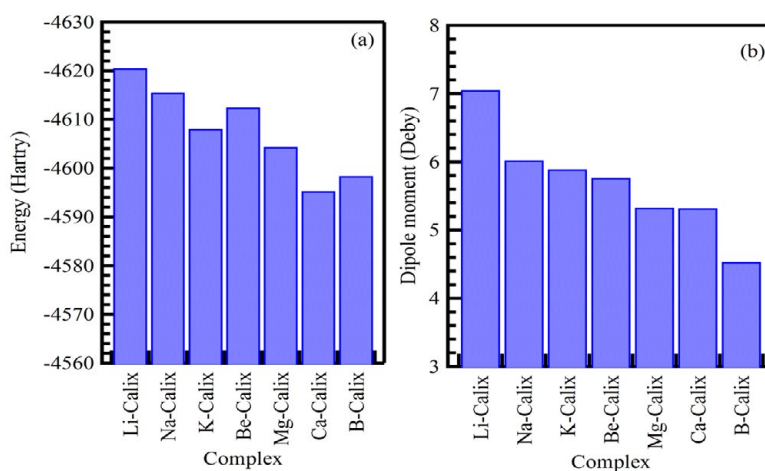


Fig. 6: Energy (a) dipole moment (b) vs. calix[8]arene complexes with some metals at HF level.



## CONCLUSION

This article presents an HF study on calix[8] arene which investigated the hydrogen, oxygen and nitrogen atoms as active sites of an organic structure. The most chemical shift and the least isotropic chemical shift is related to nitrogen atoms but the total charge decrease for them. That is because of conjugated bonds and aromaticity of the nitrogen bonds configuration and the resonance occur between non-planar sheets. In addition, the most of the total charge attached to nitrogen atoms and then metal atoms is due to of electronegativity of oxygen atoms that linked to them.

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## CONFLICT OF INTEREST

All authors declare no conflicts of interest in this paper.

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