



# Computing Group Theory and Character Table of Non Rigid Tetraphenylporphyrin H<sub>2</sub> (Tpp) and Metalloporphyrin Mii (Tpp)

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# Computing Group Theory and Character Table of Non Rigid Tetraphenylporphyrin H<sub>2</sub> (Tpp) and Metalloporphyrin M<sup>II</sup> (Tpp)

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**Abstract** - The studies on symmetry of Metalloporphyrins are very important due to better understanding of their spectra. Also, the non rigid molecule group theory, in which the dynamical symmetry operations are defined as physical operations, is a new field of chemistry. In this paper, by a simple method, we calculate character table for symmetry group of non rigid porphyrin molecule consisting of four phenyl groups attached to a rigid framework. We apply the group theory package, GAP, to compute the symmetry of Tetraphenylporphyrin, H<sub>2</sub>(TPP), and Metalloporphyrin, M<sup>II</sup>(TPP), with symmetry groups D<sub>2h</sub> and D<sub>4h</sub>, respectively. We prove that the full non rigid of these molecules are seen be the group of order 64 which has 16 conjugacy classes and order 128 which has 20 conjugacy classes, respectively.

**Keywords** : Character table; Conjugacy classes; GAP; Non-rigid group; Tetraphenylporphyrin.

## I. INTRODUCTION

The study of porphyrins has received increased interest in recent years. Metalloporphyrin complexes play significant roles in many biological and catalytic systems. The diversity of their functions is due in part to the variety of metals that bind in the "pocket" of the porphyrin ring system. The study of porphyrins is well suited to college and university laboratories because of their importance and several other reasons. Specifically, interpretation of their spectra offers an introduction to molecular orbital and molecular symmetry (1,2). Group theory for non-rigid molecules is becoming increasingly relevant and its numerous applications to vibrational spectroscopy of small molecules are appearing in the literatures (3,9). As it is well known, group theory for non-rigid molecules was essentially developed for two points of view: i) The molecular symmetry group theory (MSG) of permutation inversion groups constructed by permutations and permutation-inversions of identical particles (The MSG group is formed by all feasible permutations); ii) The full and restricted non-rigid group

theory built up with physical operations, expressed in terms of internal coordinates that transform one conformation into another iso-energetic one (10).

In a series of paper Ashrafi and coauthors computed full non-rigid groups of some molecules such as tetraammine platinum(II) (11), cis- and transdichlorodiammine platinum(II) and trimethylamine (12), tetraammine platinum(II) with C<sub>2v</sub> and C<sub>4v</sub> point group (13,14), tetraamine platinum(II) as a wreath product (15), tetra-tertbutyltetrahedrane (16), tetramethylethylene (17), hexamethylbenzene (18) and melamine (19).

In this paper the full non-rigid groups of Tetraphenylporphyrin, H<sub>2</sub>(TPP), and Metalloporphyrin, M<sup>II</sup>(TPP), are computed. Firstly, the algebraic structures of the full non-rigid group of these molecules are specified. Then, based on the structure of the group, a useful programming language, namely GAP (20), is applied and the character Tables of f-NRG of these molecules are computed. The GAP package is used to find many properties of the groups (21,22). We determine the order of the f-NRG of two porphyrin molecules and conjugacy classes of them. Finally, we calculate the character tables of them.

## II. THEORETICAL METHOD

Our computations were carried out using the "Groups, Algorithms and Programming" (GAP) system (20). GAP is a free and extensible software package for computation in discrete abstract algebra, in which you can write your own programs in the GAP language, and use them in the same way the programs which form part of the system are used. More information on the motivation and development of GAP to date can be found on the GAP web page (<http://www.gapsystem.org/>).

First of all, we consider the point group of Tetraphenylporphyrin, H<sub>2</sub>(TPP), and Metalloporphyrin, M<sup>II</sup>(TPP), in the case of rigid state (see Figures. 1(A) and (B) where the structures are optimized using PM3 method of the chemistry package Hyperchem (23)) and determine the point groups of full non-rigid group of these molecules with symmetry groups D<sub>2h</sub> and D<sub>4h</sub>, which denoted

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by G and K, respectively. Then we apply G and K to compute their conjugacy classes and character tables.

### III. GAP PROGRAM

The group theory of H<sub>2</sub>(TPP) and M<sup>II</sup>(TPP) can be computed using the GAP function Group() for D<sub>2h</sub> and D<sub>4h</sub> point group, respectively. Also the conjugacy classes and the character table of each of these groups can be computed using the GAP functions Conjugacy Classes() and Irr(), respectively.

### IV. RESULTS AND DISCUSSION

Determination of conjugacy classes and character table

**Tetraphenylporphyrin, H<sub>2</sub>(TPP) with D<sub>2h</sub>:** Now, we consider the point group D<sub>2h</sub> of the f-NRG of tetraphenylporphyrin. From the Figure 1(A), it follows that the elements  $\alpha_1 = (1,2)$ ,  $\alpha_2 = (3,4)$ ,  $\alpha_3 = (5,6)$  and  $\alpha_4 = (7,8)$ , which permutes hydrogens in either of phenyl cases. We assume that these operations are all feasible, that barrier to rotation of the phenyl group is low. Also there are five elements:

$$\alpha_5 = (1,5)(2,6)(3,7)(4,8)(9,13)(10,14)(11,15)(12,16),$$

$$\alpha_6 = (1,4)(2,3)(5,8)(6,7)(9,14)(10,13)(11,12)(15,16),$$

$$\alpha_7 = (1,8)(2,7)(3,6)(4,5)(9,10)(11,16)(12,15)(13,14),$$

$$\beta_1 = (1,2)(6,5),$$

$$\beta_2 = (3,4)(7,8),$$

Which correspond to C<sub>2</sub>(z), C<sub>2</sub>(y), C<sub>2</sub>(x),  $\sigma(xz)$  and  $\sigma(xy)$ , respectively. These nine permutations generate the group G and a simple GAP program shows that G is a group of order 64 with 16 conjugacy classes. The conjugacy classes of G can be computed.

The representative for conjugacy classes of G is given in Table I. Also the character table of G can be easily computed using GAP function Irr(G). From conjugacy classes of the groups G, we able to compute the irreducible character table of them. The values of the irreducible character  $\chi_i$  ( $1 \leq i \leq 16$ ) for D<sub>2h</sub> symmetry is shown in Table II.

We know the 22 p<sub>z</sub> orbitals in the free-base porphyrin are the basis of set of orbitals combined to create the  $\pi$  molecular orbitals of the porphyrin ring (1). The point group is D<sub>2h</sub>. This gives the reducible representation:

$$\begin{array}{c|cccccccc} D_{2h}(\text{rigid}) & E & C_2(z) & C_2(y) & C_2(x) & i & \sigma(xy) & \sigma(xz) & \sigma(yz) \\ \Gamma_{\text{Porphyrin}} & 22 & 0 & -2 & 0 & 0 & -22 & 0 & 2 \end{array}$$

$$\text{Which reduces to } 5B_{2g} + 6B_{3g} + 4A_u + 6B_{1u}.$$

None of these states are degenerate. But the configuration with D<sub>2h(non-rigid)</sub> symmetry possesses some rotations of phenyl groups with the symmetry representations:

$$\begin{array}{c|cccccccc} D_{2h}(\text{Non-rigid}) & 1(1a) & 4(2a) & 2(2b) & 2(2c) & 2(2d) & 4(2e) & 1(2f) & 4(2g) \\ & 8(4a) & 4(4b) & 4(2h) & 8(4c) & 4(4d) & 4(2i) & 8(4e) & 4(f) \end{array}$$

$$\begin{array}{c|cccccccccccc} \Gamma_{\text{Porphyrin}} & 22 & 22 & 22 & 22 & 22 & 22 & 22 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 2 & 2 & 2 & & & & & & & & & & \end{array}$$

$$\begin{array}{c|cccccccccccc} \Gamma_{\text{Pphenyl}} & 24 & 20 & 16 & 16 & 16 & 12 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & & & & & & & & & & \end{array}$$

Thus, the skeletal modes of a porphyrin derivative can be classified, according to the D<sub>2h</sub> symmetry, as

$$\Gamma_{\text{Ppor}} = 6\chi_1 + 6\chi_6 + 5\chi_7 + 5\chi_8$$

$$\Gamma_{\text{Pph}} = 4\chi_1 + 4\chi_6 + 4\chi_7 + 4\chi_8 + 2\chi_{16}$$

**Metalloporphyrin, M<sup>II</sup>(TPP) with D<sub>4h</sub>:** After metalation the symmetry is D<sub>4h</sub>, as all nitrogens are equivalent. Whereas during metalation the d $\pi$  metal orbital overlap with the  $\pi$  system of the porphyrin ring, the change in the porphyrin spectrum on metalation is due to increased symmetry relative to the free-base porphyrin.

Similar mentioned method, by figure 1(B) we have four rotations  $\alpha_1 = (1,2)$ ,  $\alpha_2 = (3,4)$ ,  $\alpha_3 = (5,6)$  and  $\alpha_4 = (7,8)$  in the D<sub>4h</sub> symmetry, which permutes hydrogens in either of phenyl cases. Also, we have rotation and reflections,

$$\alpha_5 = (1,3,5,7)(2,4,6,8)(9,11,13,15)(10,12,14,16),$$

$$\beta_1 = (1,2)(3,8)(4,7)(5,6)(9,12)(10,11)(13,16)(14,15),$$

$$\beta_2 = (1,6)(2,5)(3,4)(7,8)(9,16)(10,15)(11,14)(12,13),$$

$$\beta_3 = (1,4)(2,3)(5,8)(6,7)(9,14)(10,13)(11,12)(15,16),$$

$$\beta_4 = (1,8)(2,7)(3,6)(4,5)(9,10)(11,16)(12,15)(13,14),$$

for D<sub>4h</sub> point group. The permutations  $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \beta_1, \beta_2, \beta_3$  and  $\beta_4$  generate the group K. GAP program shows that K is group of order 128 with 20 conjugacy classes. The representative for conjugacy

classes and character table of **K** are shown in Table III and IV.

In rigid conformation, the resulting basis set consists of the 24  $p_z$  orbitals (1).

$$D_{4h}(\text{rigid}) \quad \left| \begin{array}{cccccccc} E & 2C_4 & C_2 & 2C_2' & 2C_2'' & i & 2S_4 & \sigma_h & 2\sigma_v & 2\sigma_v \end{array} \right.$$

$$\Gamma_{\Pi\text{porphyrin}} \quad \left| \begin{array}{cccccccc} 24 & 0 & 0 & -2 & -2 & 0 & 0 & -24 & 2 & 2 \end{array} \right.$$

Which reduces to  $6E_g + 3A_{1u} + 3A_{2u} + 3B_{1u} + 3B_{2u}$ .

But the configuration with  $D_{4h}(\text{non-rigid})$  symmetry possesses some rotations of phenyl groups with the symmetry representations:

$$D_{4h}(\text{non-rigid}) \quad \left| \begin{array}{cccccccc} 1(1a) & 4(2a) & 4(2b) & 2(2c) & 4(2d) & 4(2e) & 4(4a) & 8(2f) \\ 8(4b) & 1(2g) & 4(2h) & 4(4c) & 8(2i) & 16(4d) & 8(4e) & 16(4f) & 16(8a) & 4(2j) \\ 8(4g) & 4(4h) & & & & & & & & \end{array} \right.$$

$$\Gamma_{\Pi\text{porphyrin}} \quad \left| \begin{array}{cccccccc} 24 & 24 & 24 & 24 & 24 & 2 & 2 & 2 & 2 & 24 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & & & & & \end{array} \right.$$

$$\Gamma_{\Pi\text{phenyl}} \quad \left| \begin{array}{cccccccc} 24 & 20 & 16 & 16 & 12 & 4 & 4 & 4 & 4 & 8 & 4 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & & & & \end{array} \right.$$

$$\Gamma_{\Pi\text{por}} = 4\chi_1 + 2\chi_6 + 3\chi_7 + 3\chi_8 + 6\chi_9$$

$$\Gamma_{\Pi\text{ph}} = 3\chi_1 + \chi_6 + \chi_7 + 3\chi_8 + 4\chi_9 + \chi_{19} + \chi_{20}$$

We know the change in the spectrum on metalation is due to increased symmetry relative to the free-base porphyrin. The two hydrogens on the nitrogen atoms in the free base porphyrin reduce the ring symmetry from square (for Metalloporphyrins) to rectangular- that is from  $D_{4h}$  to  $D_{2h}$ . In general, a more symmetrical molecule gives a simpler spectrum.

## V. CONCLUSIONS

The method described in this paper appears to be more efficient in dealing with the construction to the character table of the symmetry group of the molecule. First, all the permutations and inversions which don't change the whole framework of the molecule should be examined. We have considered the point groups of Tetraphenylporphyrin,  $H_2(TPP)$ , and Metalloporphyrin,  $M^{II}(TPP)$ , in the case of non-rigid state and calculated the conjugacy classes of full non-rigid groups of  $H_2(TPP)$  and  $M^{II}(TPP)$  with symmetry groups  $D_{2h}$  and  $D_{4h}$  which denoted by **G** and **K**, respectively. Then using the **GAP** package the character table of the **f-NRG** group is computed. This method is usually very useful for calculating symmetries of the molecule, when the numbers of vertices are at most 30. It is hoped that the present study would help to interpret Raman and IR spectra of full non-rigid porphyrin derivatives and

another molecules in future.

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Table I

The representatives of conjugacy classes of the group G (D<sub>2h</sub>)

No.	Representative	Size	Name	Symmetry
1	()	1	1a	<i>E</i>
2	(7,8)	4	2a	$\alpha_4$
3	(5,6)(7,8)	2	2b	$\alpha_3\alpha_4$
4	(3,4)(7,8)	2	2c	$\alpha_2\alpha_4$
5	(3,4)(5,6)	2	2d	$\alpha_2\alpha_3$
6	(3,4)(5,6)(7,8)	4	2e	$\alpha_2\alpha_3\alpha_4$
7	(1,2)(3,4)(5,6)(7,8)	1	2f	$\alpha_1\alpha_2\alpha_3\alpha_4$
8	(1,3)(2,4)(5,7)(6,8)(9,14)(10,13)(11,12)(15,16)	4	2g	$\alpha_1\alpha_2\alpha_3\beta_1\alpha_3$
9	(1,3)(2,4)(5,7,6,8)(9,14)(10,13)(11,12)(15,16)	8	4a	$\alpha_1\alpha_2\alpha_3\beta_1$
10	(1,3,2,4)(5,7,6,8)(9,14)(10,13)(11,12)(15,16)	4	4b	$\alpha_1\alpha_3\beta_1$
11	(1,5)(2,6)(3,7)(4,8)(9,13)(10,14)(11,15)(12,16)	4	2h	$\alpha_5$
12	(1,5)(2,6)(3,7,4,8)(9,13)(10,14)(11,15)(12,16)	8	4c	$\alpha_5\alpha_2$
13	(1,5,2,6)(3,7,4,8)(9,13)(10,14)(11,15)(12,16)	4	4d	$\alpha_3\alpha_5\alpha_2$
14	(1,7)(2,8)(3,5)(4,6)(9,10)(11,16)(12,15)(13,14)	4	2i	$\alpha_1\alpha_2\alpha_3\beta_2\alpha_1$
15	(1,7,2,8)(3,5)(4,6)(9,10)(11,16)(12,15)(13,14)	8	4e	$\alpha_1\alpha_2\alpha_3\beta_2$
16	(1,7,2,8)(3,5,4,6)(9,10)(11,16)(12,15)(13,14)	4	4f	$\alpha_1\alpha_2\beta_2$

Table II

The representatives of conjugacy classes of the group K (D<sub>4h</sub>)

No.	Representative	Size	Name	Symmetry
1	()	1	1a	<i>E</i>
2	(7,8)	4	2a	$\alpha_4$
3	(5,6)(7,8)	4	2b	$\alpha_3\alpha_4$
4	(3,4)(7,8)	2	2c	$\alpha_2\alpha_4$
5	(3,4)(5,6)(7,8)	4	2d	$\alpha_2\alpha_3\alpha_4$
6	(3,7)(4,8)(9,12)(10,11)(13,16)(14,15)	4	2e	$\alpha_1\alpha_2\alpha_3\alpha_4\beta_1$
7	(3,7,4,8)(9,12)(10,11)(13,16)(14,15)	4	4a	$\alpha_1\alpha_2\alpha_3\beta_1$
8	(3,7)(4,8)(5,6)(9,12)(10,11)(13,16)(14,15)	8	2f	$\alpha_1\alpha_2\alpha_4\beta_1$
9	(3,7,4,8)(5,6)(9,12)(10,11)(13,16)(14,15)	8	4b	$\alpha_1\alpha_2\beta_1$
10	(1,2)(3,4)(5,6)(7,8)	1	2g	$\alpha_1\alpha_2\alpha_3\alpha_4$
11	(1,2)(3,7)(4,8)(5,6)(9,12)(10,11)(13,16)(14,15)	4	2h	$\alpha_2\alpha_4\beta_1$
12	(1,2)(3,7,4,8)(5,6)(9,12)(10,11)(13,16)(14,15)	4	4c	$\alpha_2\beta_1$
13	(1,3)(2,4)(5,7)(6,8)(9,14)(10,13)(11,12)(15,16)	8	2i	$\alpha_1\alpha_2\alpha_3\alpha_4\beta_3$
14	(1,3)(2,4)(5,7,6,8)(9,14)(10,13)(11,12)(15,16)	16	4d	$\alpha_1\alpha_2\alpha_3\beta_3$



15	(1,3,2,4)(5,7,6,8)(9,14)(10,13)(11,12)(15,16)	8	4e	$\alpha_1\alpha_3\beta_3$
16	(1,3,5,7)(2,4,6,8)(9,11,13,15)(10,12,14,16)	16	4f	$\alpha_5$
17	(1,3,5,7,2,4,6,8)(9,11,13,15)(10,12,14,16)	16	8a	$\alpha_4\alpha_5$
18	(1,5)(2,6)(3,7)(4,8)(9,13)(10,14)(11,15)(12,16)	4	2j	$\alpha_5^2$
19	(1,5)(2,6)(3,7,4,8)(9,13)(10,14)(11,15)(12,16)	8	4g	$\alpha_4\alpha_5^2$
20	(1,5,2,6)(3,7,4,8)(9,13)(10,14)(11,15)(12,16)	4	4h	$\alpha_3\alpha_4\alpha_5^2$

Table III

The character table of the group G ( $D_{2h}$ )

$D_{2h}$	1a	2a	2b	2c	2d	2e	2f	2g	4a	4b	2h	4c	4d	2i	4e	4f
$\chi_1$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
$\chi_2$	1	-1	1	1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
$\chi_3$	1	-1	1	1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
$\chi_4$	1	-1	1	1	1	-1	1	1	-1	1	-1	1	-1	-1	1	-1
$\chi_5$	1	-1	1	1	1	-1	1	1	-1	1	1	-1	1	1	-1	1
$\chi_6$	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$\chi_7$	1	1	1	1	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$\chi_8$	1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$\chi_9$	2	0	-2	2	-2	0	2	0	0	0	-2	0	2	0	0	0
$\chi_{10}$	2	0	-2	2	-2	0	2	0	0	0	2	0	-2	0	0	0
$\chi_{11}$	2	0	-2	-2	2	0	2	0	0	0	0	0	0	-2	0	2
$\chi_{12}$	2	0	-2	-2	2	0	2	0	0	0	0	0	0	2	0	-2
$\chi_{13}$	2	0	2	-2	-2	0	2	-2	0	2	0	0	0	0	0	0
$\chi_{14}$	2	0	2	-2	-2	0	2	2	0	-2	0	0	0	0	0	0
$\chi_{15}$	4	-2	0	0	0	2	-4	0	0	0	0	0	0	0	0	0
$\chi_{16}$	4	2	0	0	0	-2	-4	0	0	0	0	0	0	0	0	0

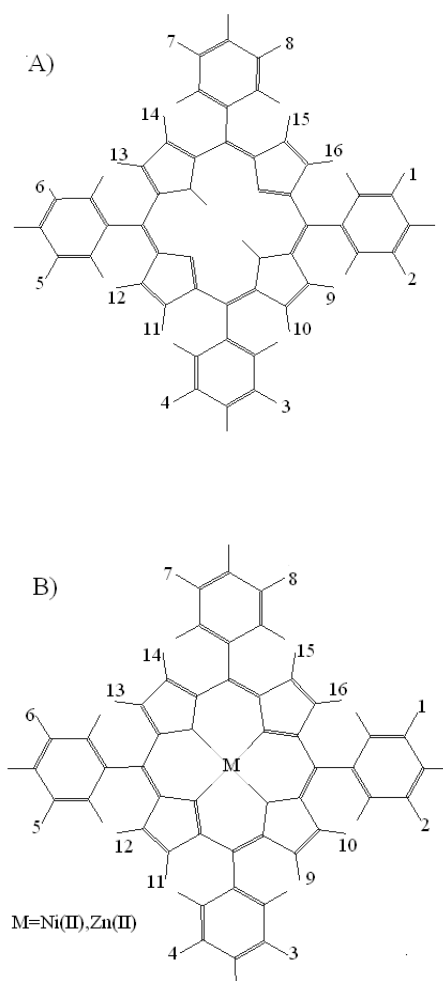


Table IV

The character table of the group K ( $D_{4h}$ )

$D_{4h}$	1a	2a	2b	2c	2d	2e	4a	2f	4b	2g	2h	4c	2i	4d	4e	4f	8a	2j	4g	4h
$\chi_1$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
$\chi_2$	1	-1	1	1	-1	-1	1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
$\chi_3$	1	-1	1	1	-1	-1	1	1	-1	1	-1	1	1	-1	1	-1	1	1	-1	1
$\chi_4$	1	-1	1	1	-1	1	-1	-1	1	1	1	-1	-1	1	-1	-1	1	1	-1	1
$\chi_5$	1	-1	1	1	-1	1	-1	-1	1	1	1	-1	1	-1	1	1	-1	1	-1	1
$\chi_6$	1	1	1	1	1	-1	-1	-1	-1	1	-1	-1	-1	-1	-1	1	1	1	1	1
$\chi_7$	1	1	1	1	1	-1	-1	-1	-1	1	-1	-1	1	1	1	-1	-1	1	1	1
$\chi_8$	1	1	1	1	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	1	1	1
$\chi_9$	2	2	2	2	2	0	0	0	0	2	0	0	0	0	0	0	0	-2	-2	-2
$\chi_{10}$	2	-2	2	2	-2	0	0	0	0	2	0	0	0	0	0	0	0	-2	2	-2
$\chi_{11}$	2	0	-2	2	0	2	0	0	-2	2	2	0	0	0	0	0	0	2	0	-2
$\chi_{12}$	2	0	-2	2	0	-2	0	0	2	2	-2	0	0	0	0	0	0	2	0	-2
$\chi_{13}$	2	0	-2	2	0	0	-2	2	0	2	0	-2	0	0	0	0	0	-2	0	2
$\chi_{14}$	2	0	-2	2	0	0	2	-2	0	2	0	2	0	0	0	0	0	-2	0	2
$\chi_{15}$	4	0	0	-4	0	0	0	0	0	4	0	0	-2	0	2	0	0	0	0	0
$\chi_{16}$	4	0	0	-4	0	0	0	0	0	4	0	0	2	0	-2	0	0	0	0	0
$\chi_{17}$	4	-2	0	0	2	-2	2	0	0	-4	2	-2	0	0	0	0	0	0	0	0
$\chi_{18}$	4	-2	0	0	2	2	-2	0	0	-4	-2	2	0	0	0	0	0	0	0	0
$\chi_{19}$	4	2	0	0	-2	-2	-2	0	0	-4	2	2	0	0	0	0	0	0	0	0
$\chi_{20}$	4	2	0	0	-2	2	2	0	0	-4	-2	-2	0	0	0	0	0	0	0	0





*Figure 1.* Top-view diagram of the structures of (A) Tetraphenylporphyrin, H<sub>2</sub>(TPP), and (B) Metalloporphyrin, M<sup>II</sup>(TPP).





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