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Toxicity Analysis of Polychlorinated Dibenzofurans through Global and Local Electrophilicities

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Abstract

Toxicity of polychlorinated dibenzofurans are correlated with global and local electrophilicities calculated through DFT/6-31G(d) method with B3LYP functionals using both Mulliken and Hirshfeld population analysis schemes. An excellent correlation is observed between the experimental binding affinity values of 31 polychlorinated dibenzofurans with AhR receptors and a linear combination of global and local electrophilicity values.

Motivation. To verify the importance of global and local electrophilicities in analyzing toxicity within a QSAR parlance.

Method. Calculation ω and ω_k^+ of 31 polychlorinated dibenzofurans using Becke's three parameter hybrid density functional, B3LYP, with 6-31G(d) basis set and Mulliken and Hirshfeld population analysis schemes.

Results. A linear relation between the experimental binding affinities (pIC_{50}) of polychlorinated biphenyls with biosystems and a linear combination of global and local electrophilicity values is observed.

Conclusions. The global and local electrophilicities together can explain the toxicities of polychlorinated dibenzofurans. The beautiful correlation between the binding affinity of these toxins with biosystems and a linear combination of global and local electrophilicity values confirms the importance of charge transfer in analyzing the origin of toxicity.

Keywords. DFT, Dibenzofuran, Toxicity,Electrophilicity.

Abbreviations and notations

QSAR, Quantitative Structure Activity Relationship
DFT, Density Functional Theory
HAH, Halogenated aromatic hydrocarbon
PCDF, Polychlorinated Dibenzofuran
FF, Fukui Function
IP, Ionization Potential
EA, Electron Affinity
HOMO, Highest Occupied Molecular Orbital
LUMO, Lowest Unccupied Molecular Orbital

Dedicated to Professor Danail Bonchev on his 65th birthday

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1 INTRODUCTION

Halogenated aromatic hydrocarbons (HAH) like polychlorinated biphenyls, dibenzo-p-dioxins, dibenzofurans and benzidines exhibit toxic behavior mainly through their interaction with the biological systems essentially via a protein called AhR [1-3]. Several studies on these compounds have been performed [4-10] in order to gain insights into the actual nature of binding between the HAH and AhR. The interaction is mainly through partial charge transfer augmented by π- stacking and in most cases the toxins (HAH) behave as electron acceptors which forces us to treat the electrophilicity as the natural reactivity descriptor [7-9] in the associated quantitative structure activity relationships (QSAR). The amount of charge transfer and the direction of charge flow between the toxin and the biosystem also provide [7-9] important insights into the associated toxicity.

Halogenated aromatic hydrocarbons (HAH) like dibenzofuran occur predominantly as industrial byproducts and the genesis of their toxicity is very complicated and is yet to be understood clearly. Because of the experimental difficulties related to the study of these halogenated aromatic hydrocarbons, QSAR would be helpful to correlate the biological and toxicological activities of these HAHs with different reactivity descriptors.

Compounds are generally screened on the computer in order to select structure with the desired properties using correlation between the structure and the activity of these compounds in QSAR. But it is quite difficult to find good correlation between structure and activity though there exist several models in QSAR. In recent years quantum chemical descriptors are used in QSAR studies because the quantum chemical quantities are able to provide accurate quantitative description of the molecular structures and their chemical properties. Atomic charges, molecular orbital energies, frontier orbital densities, atom- atom polarizabilites, molecular polarizabilities, dipole moments etc., have been used as descriptors within a QSAR parlance.

In the present study we have used global and local electrophilicities as descriptors. According to the density functional theory (DFT) the chemical potential (μ), and chemical hardness (η) are defined as,

$$\chi = -\mu = -\left(\frac{\partial E}{\partial N}\right)_{v(\vec{r})} \tag{1}$$

and

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{v(\vec{r})} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_{v(\vec{r})} \tag{2}$$

where E is the total energy of the system, N is the number of electrons in the system and $v(\vec{r})$ is the external potential.

The vertical ionization potential (IP) of a system is the change of energy when an electron is removed from the system and variation of the energy when an electron is added to the system is known as electron affinity (EA). In both the cases, electron withdrawing and electron addition, the external potential has to be kept fixed. So using finite difference approximation, eqns. (1) and (2) become,

$$\mu = -\frac{(IP+EA)}{2} \tag{3}$$

$$\eta = \frac{IP-EA}{2} \tag{4}$$

However, to obtain the IP and EA and hence μ and η, one needs three energy values (E_N, E_{N+1} and E_{N-1}). To save the computational time, we have calculated chemical potential and chemical hardness by using Koopmans' theorem as,

$$\mu = \frac{E_{LUMO}+E_{HOMO}}{2} \tag{5}$$

and

$$\eta = \frac{E_{LUMO}-E_{HOMO}}{2} \tag{6}$$

where E_{LUMO} is the lowest unoccupied molecular orbital's energy and E_{HOMO} is the highest occupied molecular orbital's energy.

Using μ and η Parr *et al* have defined a new quantum chemical descriptor, known as electrophilicity index (ω) which measures the propensity to absorb electrons and is defined as [11]

$$\omega = \frac{\mu^2}{2\eta} \tag{7}$$

The Fukui function is defined within a DFT framework as [12],

$$f(\vec{r}) = \left(\frac{\partial\rho(\vec{r})}{\partial N}\right)_{v(\vec{r})} = \left(\frac{\delta\mu}{\delta v(\vec{r})}\right)_N \tag{8}$$

where $\rho(\vec{r})$ is the electron density.

Recently Chattaraj *et al* provide [13, 14] a unified treatment of chemical reactivity and selectivity through a generalized philicity concept by using a resolution of identity. This local philicity index is given as

$$\omega^{\alpha}(\vec{r}) = \omega f^{\alpha}(\vec{r}) \tag{9}$$

or its condensed- to- atom variants for the atomic site *k* in a molecule is defined as

$$\omega_k^{\alpha} = \omega f_k^{\alpha} \tag{10}$$

where $\alpha = +,-,0$ refer to nucleophilic, electrophilic and radical attacks respectively where f_k^{α} is the corresponding Fukui function.

In the present work an attempt has been made in correlating the binding affinities of 31 polychlorinated dibenzofurans in terms of their global and local electrophilicity values.

2 COMPUTATIONAL DETAILS

All the structures of the polychlorinated dibenzofurans are optimized to their lowest energy states using the Gaussian 03 software package. During the process of optimization no symmetry restriction has been made use of. The frequency calculation has been followed by the optimization procedure. The presence of zero imaginary frequency in the frequency calculation on the optimized geometries confirms that the structures are minima on the potential energy surface and hence the lowest energy ground states. Becke's three- parameter hybrid density functional, B3LYP, with basis set 6-31G(d) has been used. Fukui functions have been calculated using the direct method proposed by Contreras et al [15] and using the Mulliken population analysis (MPA) scheme as well as with the Hirshfeld population analysis (HPA) scheme [16] using DMOL package [17] with BLYP/DN method.

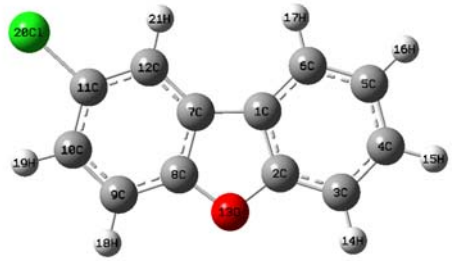
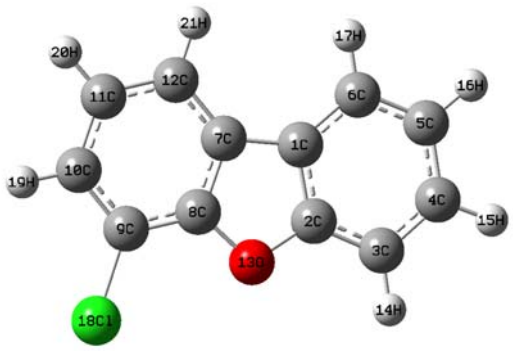
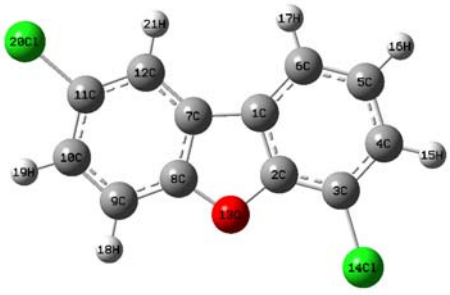
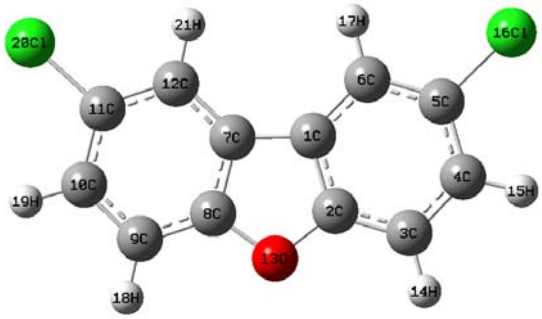
3 RESULTS AND DISCUSSION

Optimized structures with the atom- numbering schemes of all the polychlorinated dibenzofurans (PCDF) studied in the present work are provided in Figure 1 whereas their geometrical parameters are presented in Table 1. In our previous works [7-9] related to the effect of conformational flexibility on toxicity of polychlorinated biphenyls and benzdines, we highlighted the importance of the global electrophilic behavior characterized by ω as well as that of the most probable site given by ω_k^{α}. Table 2 reports the total energy, hardness, chemical potential, global electrophilicity and the local electrophilicity (both MPA and HPA) for the centre with the maximum value. In order to ascertain the actual direction of the charge transfer we have also presented the hardness, chemical potential and global electrophilicity of the selected nucleic acid (NA) bases (adenine, thymine, guanine, cytosine and urasil) and DNA base pairs (GCWC, ATH) in Table 3. Since electrons flow from a system of higher chemical potential (lower electronegativity) to another of lower chemical potential (higher electronegativity) PCDFs will act as electron acceptors and the bases/base pairs as electron donors. An analysis of the joint hardness ($\eta_{AB} = \frac{IP_{\min} - EA_{\max}}{2}$) also provides (not shown here) the same inference. Therefore we have to take ω_k^{+} (k is the site having the maximum ω^{+} value) into consideration. In case the toxin is an electron donor (like benzidines) we should consider ω_k^{-}. It is imperative to develop a QSAR based on two related parameters, one global (ω) and one local (ω_k^{+} for electron acceptors and ω_k^{-} for electron donors). Figure 2 shows the excellent correlation between the observed binding affinity (BA) of the toxins with AhR receptors [4, 5] in terms of their [pIC_{50}= -log(IC_{50})] values where IC_{50} is the inhibitor concentration [6] needed to reduce the enzyme activity by 50% and the corresponding calculated BA values in terms of ω and ω_k^{+}. The correlation is very good in the cases of the local descriptors calculated using HPA (R=0.8742, fig. 2a) and MPA (R=0.8184, fig. 2b) and also by using the BA values normalized [6] to that of 2, 3, 7, 8- tetrachloro dibenzofuran (TCDF) (figs. 2c (R=0.8722,HPA) and 2d (R=0.8157, MPA)). These correlations are better than both one and multi- parameter fits reported in reference 10. Incidentally their [10] finding of reliability of softness as the toxicity descriptor is a manifestation of the maximum hardness principle [18] as was highlighted in the toxicity analysis of polychlorinated biphenyls [7, 8] and benzidine [9] The superiority of the present QSAR not only rests on better regression but also on the transparent understanding of the DFT-based global and local reactivity descriptors used here vis- á- vis the importance of the electron

transfer ability between a toxin and a biosystem in gaining insights into the overall toxicity. Further work along this line is in progress in our laboratories.

4. Conclusions

Since the toxicity of halogenated aromatic hydrocarbons mainly originates from their interaction with biosystems essentially through electron transfer it is expected that global and local electrophilicities would provide important insights into their toxic behavior. An excellent linear correlation between the binding affinity of polychlorinated dibenzofurans with AhR receptors and a linear combination of global and local electrophilicities is observed. The genesis of this beautiful quantitative structure activity relationship is also now well understood.

1 	2 
3 	4 
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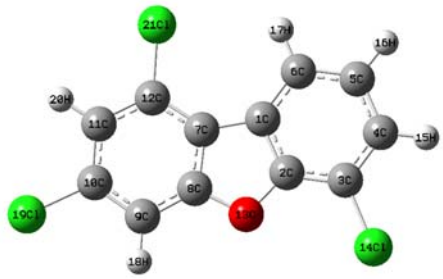

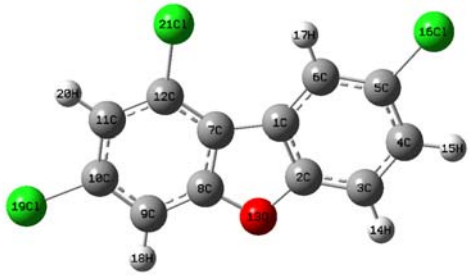

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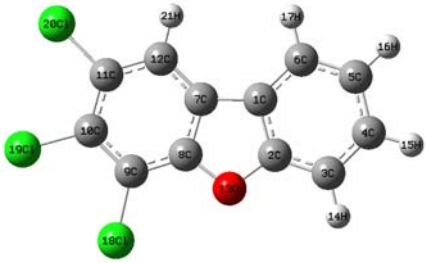

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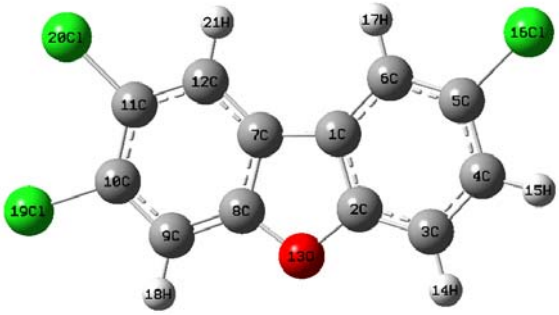

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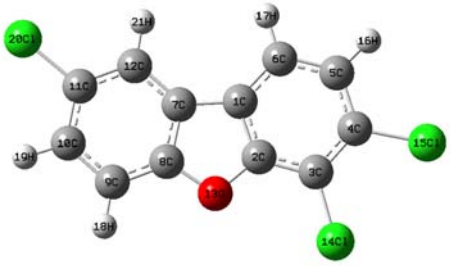

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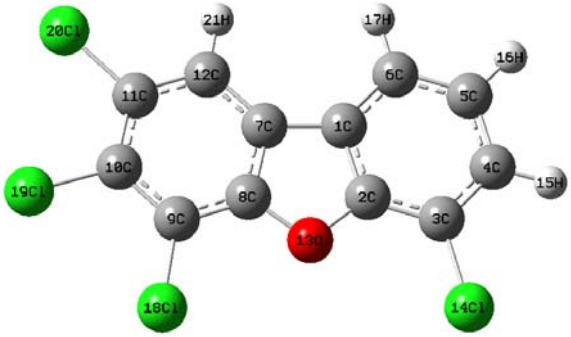

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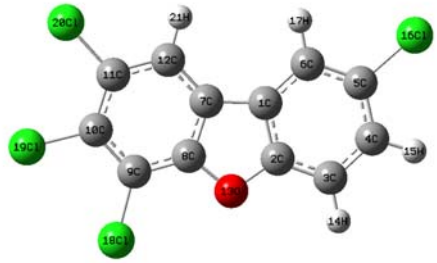

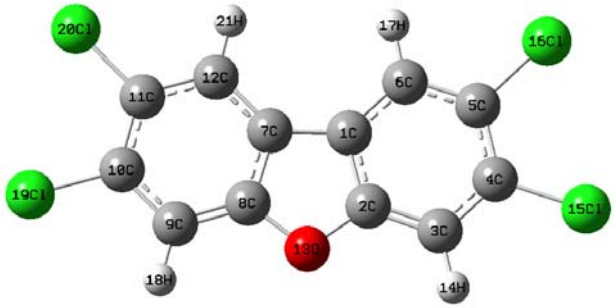

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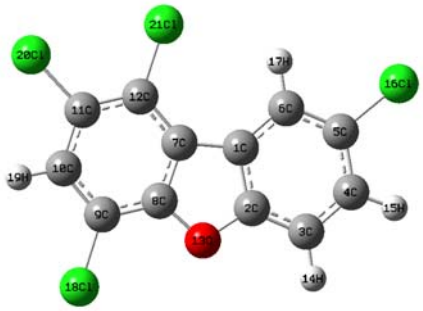

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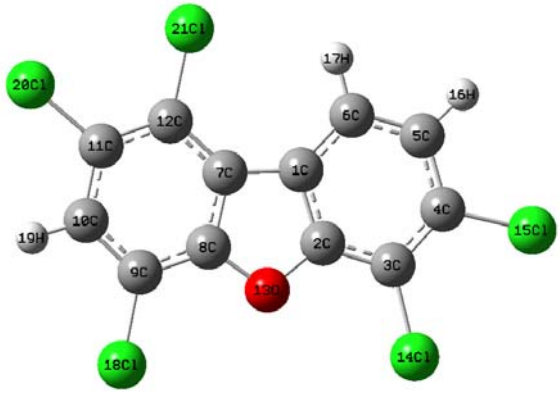

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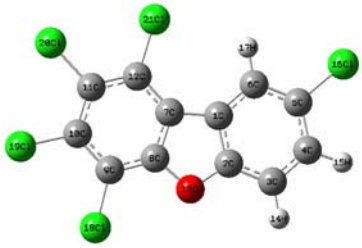

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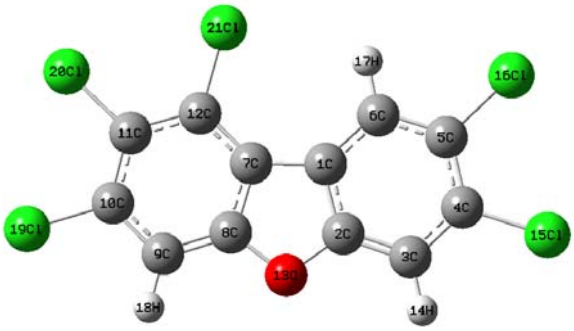

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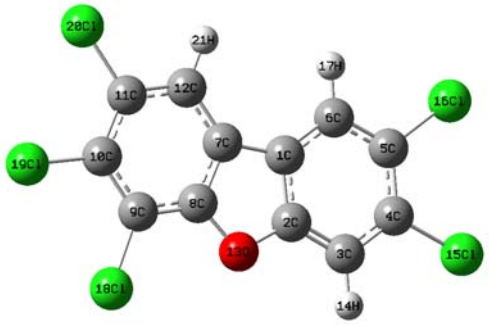

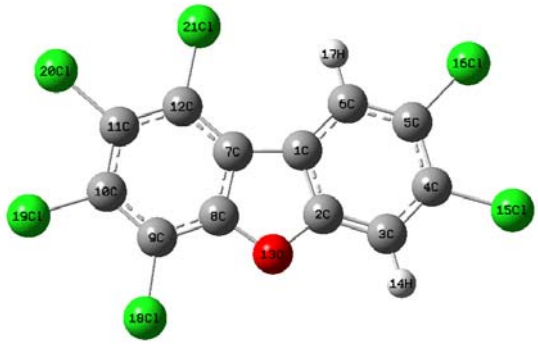

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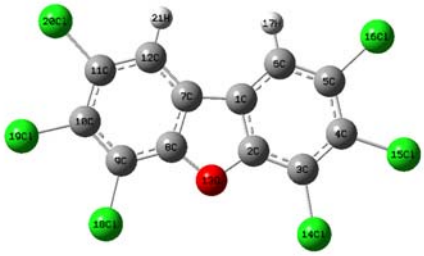

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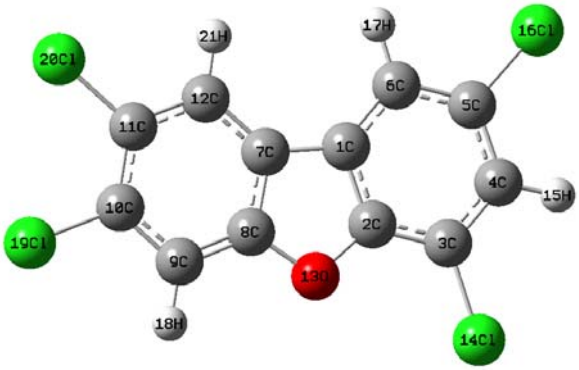

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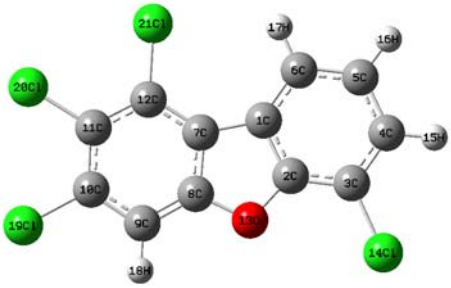

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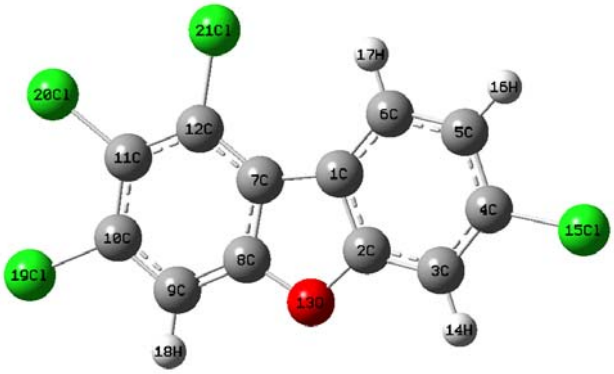

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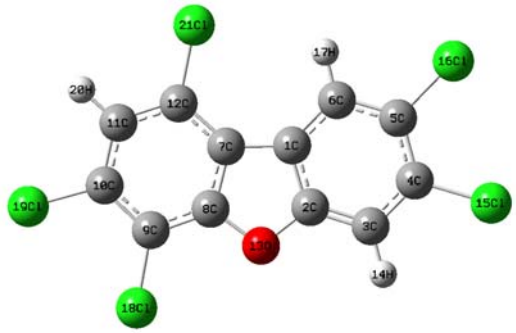

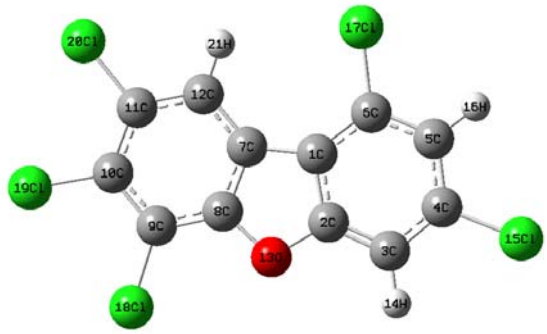

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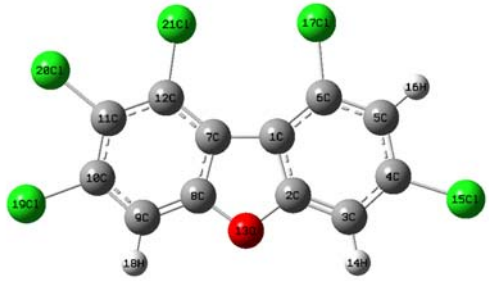

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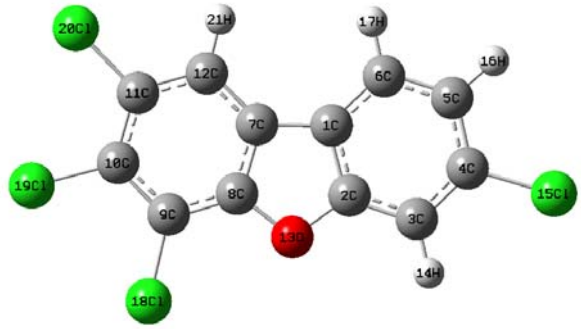

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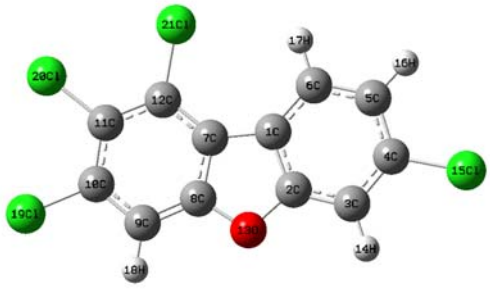

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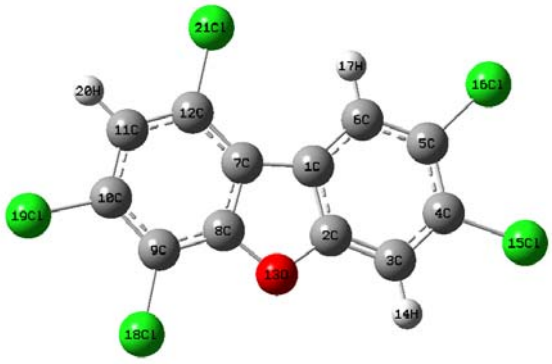

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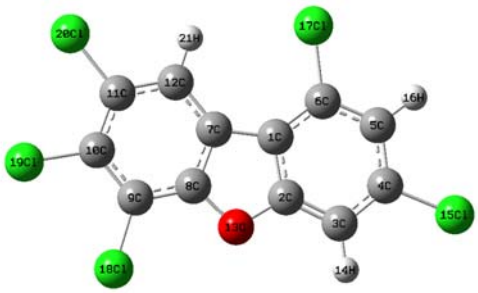

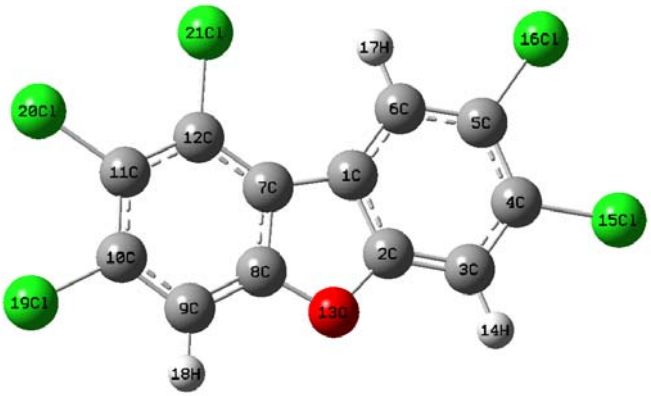

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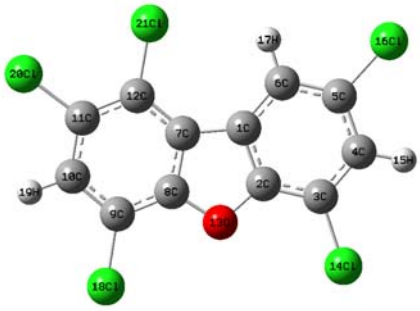
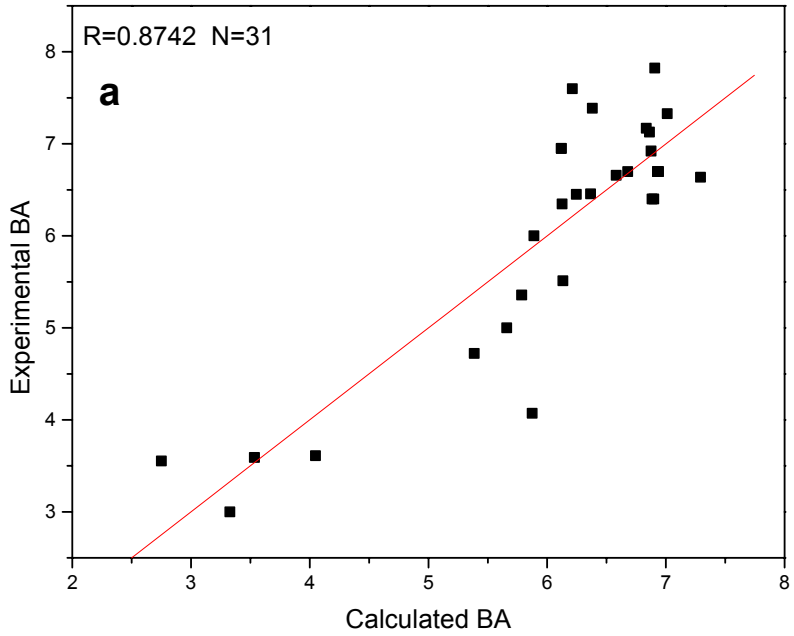
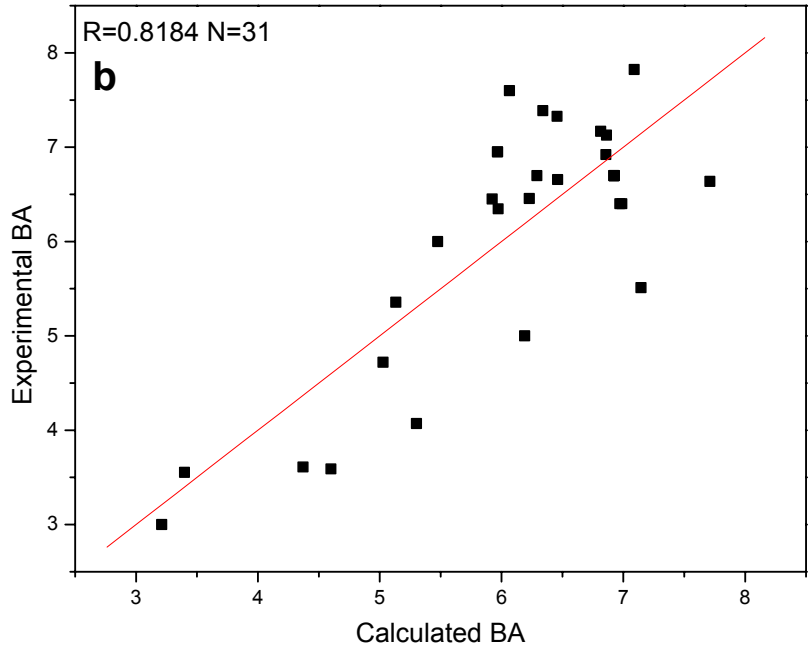


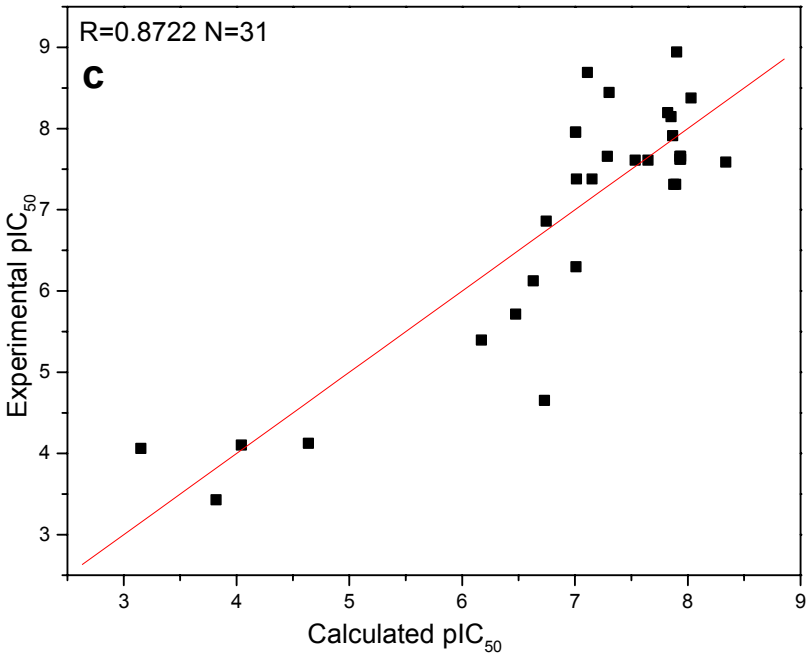
Figure 1. Geometries of different polychlorinated dibenzofurans with atom numbering



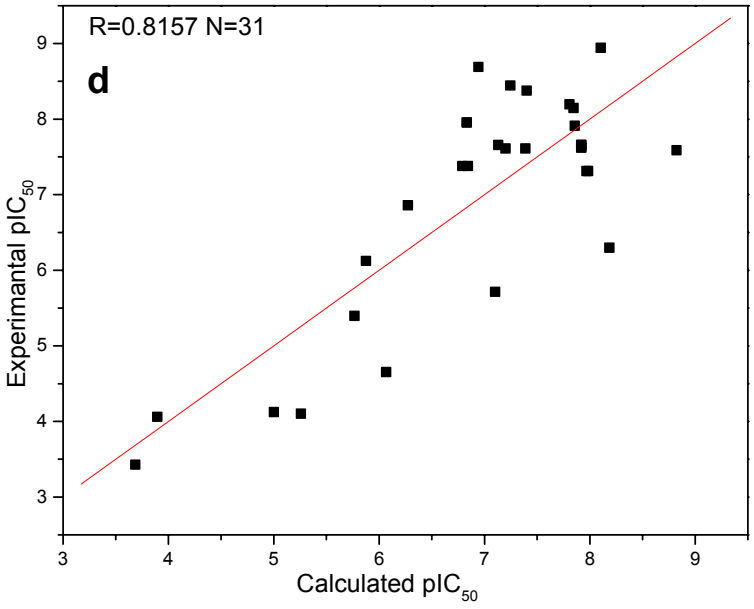
Calculated BA= -3.8314 + 613.4692*ω + 15.1564* ω^{+}_{max}



Calculated BA = -4.5426 - 3.4852*ω + 78.7406* ω^{+}_{max}



Calculated pIC_{50}= -4.3483 + 16.6328*ω + 706.8821* ω^{+}_{max}



Calculated pIC_{50}= -5.1966 + 88.2057*ω+ 8.5797* ω^{+}_{max}

Figure 2. Correlation between calculated and experimental binding affinities (pIC_{50}): a) HPA, b) MPA; corresponding values normalized to that of (TCDF) c) HPA, d) MPA.

Acknowledgments

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5 References

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Table 1: Geometrical Parameters of Different Polychlorinated Dibenzofurans

Molecule	Bond Length (A)	Angle (Degree)	Dihedral Angle (Degree)
1	C2-C1=1.408 C3-C2=1.388 C4-C3=1.396 C5-C4=1.405 C6-C5=1.393 C7-C1=1.452 C8-C7=1.408 C9-C8=1.387 C10-C9=1.395 C11-C10=1.403 C12-C11=1.392 O13-C8=1.375 H14-C3=1.085 H15-C4=1.086 H16-C5=1.086 H17-C6=1.086 H18-C9=1.085 H19-C10=1.084 Cl20-C11=1.762 H21-C12=1.085	C3-C2-C1=123.309 C4-C3-C2=116.627 C5-C4-C3=121.370 C6-C5-C4=121.069 C7-C1-C6=135.620 C8-C7-C1=105.408 C9-C8-C7=123.095 C10-C9-C8=117.147 C11-C10-C9=120.301 C12-C11-C10=122.380 O13-C8-C7 =111.693 H14-C3-C2=121.190 H15-C4-C3=119.194 H16-C5-C4=119.361 H17-C6-C5=120.641 H18-C9-C8=121.356 H19-C10-C9=120.215 Cl20-C11-C10=118.650 H21-Cl20-C11=120.598	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
2	C2-C1=1.407 C3-C2=1.387 C4-C3=1.396 C5-C4=1.405 C6-C5=1.394 C7-C1=1.453 C8-C7=1.409 C9-C8=1.390 C10-C9=1.394 C11-C10=1.403 C12-C11=1.393 O13-C8=1.369 H14-C3=1.085	C3-C2-C1=123.449 C4-C3-C2=116.551 C5-C4-C3=121.358 C6-C5-C4=121.098 C7-C1-C6=135.493 C8-C7-C1=104.960 C9-C8-C7=122.054 C10-C9-C8=117.911 C11-C10-C9=120.571 C12-C11-C10=121.379 O13-C8-C7 =112.137 H14-C3-C2=121.231 H15-C4-C3=119.186	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000

	H15-C4=1.086 H16-C5=1.086 H17-C6=1.086 Cl18-C9=1.748 H19-C10=1.085 H20-C11=1.086 H21-C12=1.086	H16-C5-C4=119.353 H17-C6-C5=120.641 Cl18-C9-C8=120.776 H19-C10-C9=118.997 H20-C11-C10=118.815 H21-Cl20-C11=120.682	H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 H20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
3	C2-C1=1.409 C3-C2=1.390 C4-C3=1.394 C5-C4=1.404 C6-C5=1.393 C7-C1=1.452 C8-C7=1.406 C9-C8=1.387 C10-C9=1.395 C11-C10=1.404 C12-C11=1.392 O13-C8=1.370 Cl14-C3=1.747 H15-C4=1.085 H16-C5=1.086 H17-C6=1.086 H18-C9=1.084 H19-C10=1.084 Cl20-C11=1.761 H21-C12=1.084	C3-C2-C1=122.057 C4-C3-C2=117.826 C5-C4-C3=120.643 C6-C5-C4=121.391 C7-C1-C6=135.431 C8-C7-C1=105.522 C9-C8-C7=123.215 C10-C9-C8=117.007 C11-C10-C9=120.378 C12-C11-C10=122.366 O13-C8-C7 =112.165 Cl14-C3-C2=120.784 H15-C4-C3=118.971 H16-C5-C4=118.821 H17-C6-C5=120.714 H18-C9-C8=121.394 H19-C10-C9=120.172 Cl20-C11-C10=118.655 H21-Cl20-C11=120.614	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
4	C2-C1=1.408 C3-C2=1.388 C4-C3=1.395 C5-C4=1.404 C6-C5=1.392 C7-C1=1.452 C8-C7=1.408 C9-C8=1.388 C10-C9=1.395 C11-C10=1.404 C12-C11=1.392 O13-C8=1.376 H14-C3=1.085 H15-C4=1.084 Cl16-C5=1.760 H17-C6=1.085 H18-C9=1.085 H19-C10=1.084 Cl20-C11=1.760 H21-C12=1.085	C3-C2-C1=123.074 C4-C3-C2=117.089 C5-C4-C3=120.384 C6-C5-C4=122.347 C7-C1-C6=135.171 C8-C7-C1=105.324 C9-C8-C7=123.084 C10-C9-C8=117.082 C11-C10-C9=120.387 C12-C11-C10=122.347 O13-C8-C7 =111.725 H14-C3-C2=121.377 H15-C4-C3=120.184 Cl16-C5-C4=118.656 H17-C6-C5=120.604 H18-C9-C8=121.377 H19-C10-C9=120.182 Cl20-C11-C10=118.651 H21-Cl20-C11=120.610	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
5	C2-C1=1.409 C3-C2=1.389 C4-C3=1.394 C5-C4=1.403 C6-C5=1.393 C7-C1=1.452 C8-C7=1.410 C9-C8=1.386 C10-C9=1.394 C11-C10=1.402 C12-C11=1.392 O13-C8=1.372 Cl14-C3=1.746 H15-C4=1.085 H16-C5=1.086 H17-C6=1.084 H18-C9=1.083 Cl19-C10=1.754	C3-C2-C1=122.347 C4-C3-C2=117.708 C5-C4-C3=120.559 C6-C5-C4=121.619 C7-C1-C6=135.845 C8-C7-C1=105.754 C9-C8-C7=124.455 C10-C9-C8=115.727 C11-C10-C9=122.589 C12-C11-C10=119.469 O13-C8-C7 =112.161 Cl14-C3-C2=120.821 H15-C4-C3=118.959 H16-C5-C4=118.789 H17-C6-C5=120.917 H18-C9-C8=121.992 Cl19-C10-C9=118.933 H20-C11-C10=120.253	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 H20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=180.000

	H20-C11=1.083 Cl21-C12=1.752	Cl21-Cl20-C11=119.0577	
6	C2-C1=1.408 C3-C2=1.386 C4-C3=1.395 C5-C4=1.403 C6-C5=1.392 C7-C1=1.451 C8-C7=1.410 C9-C8=1.387 C10-C9=1.394 C11-C10=1.402 C12-C11=1.392 O13-C8=1.370 H14-C3=1.084 H15-C4=1.084 Cl16-C5=1.760 H17-C6=1.083 H18-C9=1.083 Cl19-C10=1.754 H20-C11=1.083 Cl21-C12=1.752	C3-C2-C1=123.313 C4-C3-C2=117.010 C5-C4-C3=120.322 C6-C5-C4=122.507 C7-C1-C6=135.581 C8-C7-C1=105.569 C9-C8-C7=124.267 C10-C9-C8=115.797 C11-C10-C9=122.647 C12-C11-C10=119.409 O13-C8-C7 =111.483 H14-C3-C2=121.335 H15-C4-C3=120.195 Cl16-C5-C4=118.596 H17-C6-C5=120.840 H18-C9-C8=122.011 Cl19-C10-C9=118.890 H20-C11-C10=120.280 Cl21-H20-C11=119.135	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 H20-C11-C10-C9=180.000 Cl21-H20-C11-C10=180.000
7	C2-C1=1.406 C3-C2=1.387 C4-C3=1.396 C5-C4=1.405 C6-C5=1.393 C7-C1=1.452 C8-C7=1.406 C9-C8=1.390 C10-C9=1.406 C11-C10=1.414 C12-C11=1.392 O13-C8=1.367 H14-C3=1.085 H15-C4=1.086 H16-C5=1.086 H17-C6=1.0864 Cl18-C9=1.736 Cl19-C10=1.737 Cl20-C11=1.749 H21-C12=1.084	C3-C2-C1=123.479 C4-C3-C2=116.451 C5-C4-C3=121.421 C6-C5-C4=121.131 C7-C1-C6=135.586 C8-C7-C1=105.190 C9-C8-C7=122.761 C10-C9-C8=117.660 C11-C10-C9=119.799 C12-C11-C10=121.676 O13-C8-C7 =112.133 H14-C3-C2=121.273 H15-C4-C3=119.163 H16-C5-C4=119.337 H17-C6-C5=120.689 Cl18-C9-C8=119.603 Cl19-C10-C9=119.653 Cl20-C11-C10=120.384 H21-Cl20-C11=119.604	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
8	C2-C1=1.407 C3-C2=1.387 C4-C3=1.395 C5-C4=1.404 C6-C5=1.392 C7-C1=1.451 C8-C7=1.407 C9-C8=1.385 C10-C9=1.397 C11-C10=1.412 C12-C11=1.394 O13-C8=1.373 H14-C3=1.084 H15-C4=1.084 Cl16-C5=1.759 H17-C6=1.084 H18-C9=1.083 Cl19-C10=1.746 Cl20-C11=1.749 Cl21-C12=1.084	C3-C2-C1=123.127 C4-C3-C2=117.035 C5-C4-C3=120.416 C6-C5-C4=122.341 C7-C1-C6=135.237 C8-C7-C1=105.351 C9-C8-C7=123.223 C10-C9-C8=117.057 C11-C10-C9=120.967 C12-C11-C10=120.791 O13-C8-C7 =111.840 H14-C3-C2=121.373 H15-C4-C3=120.177 Cl16-C5-C4=118.665 H17-C6-C5=120.600 H18-C9-C8=121.913 Cl19-C10-C9=117.984 Cl20-C11-C10=120.925 Cl21-Cl20-C11=119.450	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.00 C11-C10-C9-C8=0.00 C12-C11-C10-C9=0.00 O13-C8-C7-C1 =0.00 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=180.000
9	C2-C1=1.407 C3-C2=1.390 C4-C3=1.395	C3-C2-C1=122.259 C4-C3-C2=117.573 C5-C4-C3=120.742	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000

	C5-C4= 1.404 C6-C5=1.393 C7-C1=1.452 C8-C7=1.404 C9-C8=1.390 C10-C9=1.406 C11-C10=1.414 C12-C11=1.392 O13-C8=1.369 Cl14-C3=1.744 H15-C4=1.085 H16-C5=1.086 H17-C6=1.086 Cl18-C9=1.734 Cl19-C10=1.736 Cl20-C11=1.749 H21-C12=1.084	C6-C5-C4=121.451 C7-C1-C6=135.365 C8-C7-C1=105.299 C9-C8-C7=122.897 C10-C9-C8=117.496 C11-C10-C9=119.865 C12-C11-C10=121.688 O13-C8-C7 =112.090 Cl14-C3-C2=120.879 H15-C4-C3=118.909 H16-C5-C4=118.795 H17-C6-C5=120.781 Cl18-C9-C8=119.666 Cl19-C10-C9=119.605 Cl20-C11-C10=120.384 H21-Cl20-C11=119.638	C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
10	C2-C1=1.406 C3-C2=1.387 C4-C3=1.395 C5-C4=1.404 C6-C5=1.392 C7-C1=1.452 C8-C7=1.405 C9-C8=1.390 C10-C9=1.405 C11-C10=1.415 C12-C11=1.392 O13-C8=1.367 H14-C3=1.084 H15-C4=1.084 Cl16-C5=1.758 H17-C6=1.084 Cl18-C9=1.735 Cl19-C10=1.736 Cl20-C11=1.748 H21-C12=1.084	C3-C2-C1=123.228 C4-C3-C2=116.920 C5-C4-C3=120.470 C6-C5-C4=122.338 C7-C1-C6=135.138 C8-C7-C1=105.103 C9-C8-C7=122.770 C10-C9-C8=117.592 C11-C10-C9=119.857 C12-C11-C10=121.663 O13-C8-C7 =112.171 H14-C3-C2=121.426 H15-C4-C3=120.144 Cl16-C5-C4=118.670 H17-C6-C5=120.619 Cl18-C9-C8=119.593 Cl19-C10-C9=119.625 Cl20-C11-C10=120.391 H21-Cl20-C11=119.627	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
11	C2-C1=1.408 C3-C2=1.390 C4-C3=1.394 C5-C4=1.402 C6-C5=1.399 C7-C1=1.451 C8-C7=1.410 C9-C8=1.386 C10-C9=1.394 C11-C10=1.403 C12-C11=1.392 O13-C8=1.370 Cl14-C3=1.743 H15-C4=1.083 Cl16-C5=1.757 H17-C6=1.082 H18-C9=1.083 Cl19-C10=1.752 H20-C11=1.083 Cl21-C12=1.751	C3-C2-C1=122.169 C4-C3-C2=118.018 C5-C4-C3=119.762 C6-C5-C4=119.936 C7-C1-C6=135.388 C8-C7-C1=105.693 C9-C8-C7=124.417 C10-C9-C8=115.687 C11-C10-C9=122.625 C12-C11-C10=119.514 O13-C8-C7 =112.223 Cl14-C3-C2=120.880 H15-C4-C3=119.876 Cl16-C5-C4=118.250 H17-C6-C5=121.718 H18-C9-C8=122.020 Cl19-C10-C9=118.923 H20-C11-C10=120.219 Cl21-H20-C11=119.166	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 H20-C11-C10-C9=180.000 Cl21-H20-C11-C10=180.000
12	C2-C1=1.407 C3-C2=1.384 C4-C3=1.397 C5-C4=1.412 C6-C5=1.394 C7-C1=1.451 C8-C7=1.407 C9-C8=1.384	C3-C2-C1=123.245 C4-C3-C2=117.008 C5-C4-C3=120.997 C6-C5-C4=120.787 C7-C1-C6=135.621 C8-C7-C1=105.289 C9-C8-C7=123.284 C10-C9-C8=117.006	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000

	C10-C9=1.397 C11-C10=1.412 C12-C11=1.394 O13-C8=1.375 H14-C3=1.083 Cl15-C4=1.745 Cl16-C5=1.748 H17-C6=1.084 H18-C9=1.083 Cl19-C10=1.745 Cl20-C11=1.748 H21-C12=1.084	C11-C10-C9=120.974 C12-C11-C10=120.803 O13-C8-C7 =111.837 H14-C3-C2=121.982 Cl15-C4-C3=117.969 Cl16-C5-C4=120.931 H17-C6-C5=119.475 H18-C9-C8=121.949 Cl19-C10-C9=117.981 Cl20-C11-C10=120.919 H21-Cl20-C11=119.460	C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
13	C2-C1=1.407 C3-C2=1.387 C4-C3=1.394 C5-C4=1.404 C6-C5=1.392 C7-C1=1.453 C8-C7=1.409 C9-C8=1.390 C10-C9=1.391 C11-C10=1.403 C12-C11=1.400 O13-C8=1.365 H14-C3=1.084 H15-C4=1.084 Cl16-C5=1.759 H17-C6=1.082 Cl18-C9=1.741 H19-C10=1.083 Cl20-C11=1.747 Cl21-C12=1.741	C3-C2-C1=123.446 C4-C3-C2=116.926 C5-C4-C3=120.349 C6-C5-C4=122.518 C7-C1-C6=135.578 C8-C7-C1=105.065 C9-C8-C7=122.462 C10-C9-C8=117.788 C11-C10-C9=120.800 C12-C11-C10=121.205 O13-C8-C7 =112.087 H14-C3-C2=121.328 H15-C4-C3=120.189 Cl16-C5-C4=118.591 H17-C6-C5=120.776 Cl18-C9-C8=121.023 H19-C10-C9=119.834 Cl20-C11-C10=117.754 Cl21-Cl20-C11=121.527	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=180.000
14	C2-C1=1.406 C3-C2=1.393 C4-C3=1.401 C5-C4=1.406 C6-C5=1.389 C7-C1=1.453 C8-C7=1.408 C9-C8=1.389 C10-C9=1.392 C11-C10=1.403 C12-C11=1.400 O13-C8=1.367 Cl14-C3=1.734 Cl15-C4=1.744 H16-C5=1.084 H17-C6=1.083 Cl18-C9=1.740 H19-C10=1.083 Cl20-C11=1.746 Cl21-C12=1.741	C3-C2-C1=123.526 C4-C3-C2=116.339 C5-C4-C3=121.157 C6-C5-C4=121.419 C7-C1-C6=136.095 C8-C7-C1=105.171 C9-C8-C7=122.640 C10-C9-C8=117.609 C11-C10-C9=120.861 C12-C11-C10=121.222 O13-C8-C7 =111.953 Cl14-C3-C2=120.109 Cl15-C4-C3=120.380 H16-C5-C4=118.349 H17-C6-C5=120.304 Cl18-C9-C8=121.136 H19-C10-C9=119.785 Cl20-C11-C10=117.772 Cl21-Cl20-C11=121.595	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 H19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=180.000
15	C2-C1=1.407 C3-C2=1.386 C4-C3=1.394 C5-C4=1.404 C6-C5=1.392 C7-C1=1.453 C8-C7=1.406 C9-C8=1.389 C10-C9=1.403 C11-C10=1.417 C12-C11=1.399 O13-C8=1.364 H14-C3=1.084	C3-C2-C1=123.495 C4-C3-C2=116.876 C5-C4-C3=120.374 C6-C5-C4=122.504 C7-C1-C6=135.668 C8-C7-C1=105.246 C9-C8-C7=123.367 C10-C9-C8=117.317 C11-C10-C9=120.675 C12-C11-C10=136.017 O13-C8-C7 =112.057 H14-C3-C2=121.385 H15-C4-C3=120.188	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000

	H15-C4=1.084 Cl16-C5=1.758 H17-C6=1.082 Cl18-C9=1.733 Cl19-C10=1.735 Cl20-C11=1.738 Cl21-C12=1.741	Cl16-C5-C4=118.628 H17-C6-C5=120.760 Cl18-C9-C8=119.638 Cl19-C10-C9=119.249 Cl20-C11-C10=119.714 Cl21-Cl20-C11=119.431	H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=0.000
16	C2-C1=1.407 C3-C2=1.384 C4-C3=1.396 C5-C4=1.412 C6-C5=1.394 C7-C1=1.452 C8-C7=1.407 C9-C8=1.383 C10-C9=1.394 C11-C10=1.414 C12-C11=1.399 O13-C8=1.371 H14-C3=1.083 Cl15-C4=1.744 Cl16-C5=1.748 H17-C6=1.082 H18-C9=1.083 Cl19-C10=1.744 Cl20-C11=1.738 Cl21-C12=1.742	C3-C2-C1=123.507 C4-C3-C2=116.983 C5-C4-C3=120.870 C6-C5-C4=120.976 C7-C1-C6=136.121 C8-C7-C1=105.437 C9-C8-C7=123.798 C10-C9-C8=116.804 C11-C10-C9=121.778 C12-C11-C10=136.242 O13-C8-C7 =111.720 H14-C3-C2=121.885 Cl15-C4-C3=118.002 Cl16-C5-C4=120.844 H17-C6-C5=119.667 H18-C9-C8=121.972 Cl19-C10-C9=117.637 Cl20-C11-C10=120.253 Cl21-Cl20-C11=119.286	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.0000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.0000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=0.000
17	C2-C1=1.405 C3-C2=1.384 C4-C3=1.397 C5-C4=1.413 C6-C5=1.394 C7-C1=1.451 C8-C7=1.4054 C9-C8=1.390 C10-C9=1.406 C11-C10=1.415 C12-C11=1.392 O13-C8=1.369 H14-C3=1.083 Cl15-C4=1.744 Cl16-C5=1.747 H17-C6=1.084 Cl18-C9=1.734 Cl19-C10=1.735 Cl20-C11=1.748 H21-C12=1.084	C3-C2-C1=123.379 C4-C3-C2=116.916 C5-C4-C3=120.990 C6-C5-C4=120.828 C7-C1-C6=135.566 C8-C7-C1=105.039 C9-C8-C7=122.826 C10-C9-C8=117.535 C11-C10-C9=119.872 C12-C11-C10=121.677 O13-C8-C7 =112.178 H14-C3-C2=121.978 Cl15-C4-C3=117.996 Cl16-C5-C4=120.909 H17-C6-C5=119.496 Cl18-C9-C8=119.625 Cl19-C10-C9=119.589 Cl20-C11-C10=120.385 H21-Cl20-C11=119.635	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
18	C2-C1=1.406 C3-C2=1.384 C4-C3=1.396 C5-C4=1.412 C6-C5=1.394 C7-C1=1.452 C8-C7=1.406 C9-C8=1.389 C10-C9=1.403 C11-C10=1.417 C12-C11=1.398 O13-C8=1.366 H14-C3=1.083 Cl15-C4=1.743 Cl16-C5=1.747 H17-C6=1.082 Cl18-C9=1.733 Cl19-C10=1.735	C3-C2-C1=123.624 C4-C3-C2=116.882 C5-C4-C3=120.886 C6-C5-C4=121.000 C7-C1-C6=136.067 C8-C7-C1=105.195 C9-C8-C7=123.391 C10-C9-C8=117.273 C11-C10-C9=120.696 C12-C11-C10=136.029 O13-C8-C7 =112.050 H14-C3-C2=121.914 Cl15-C4-C3=118.028 Cl16-C5-C4=120.844 H17-C6-C5=119.674 Cl18-C9-C8=119.660 Cl19-C10-C9=119.221 Cl20-C11-C10=119.732	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=0.000

	Cl20-C11=1.738 Cl21-C12=1.740	Cl21-Cl20-C11=119.384	
19	C2-C1=1.404 C3-C2=1.390 C4-C3=1.406 C5-C4=1.4152 C6-C5=1.392 C7-C1=1.451 C8-C7=1.404 C9-C8=1.390 C10-C9=1.409 C11-C10=1.415 C12-C11=1.392 O13-C8=1.370 Cl14-C3=1.733 Cl15-C4=1.734 Cl16-C5=1.747 H17-C6=1.084 Cl18-C9=1.733 Cl19-C10=1.735 Cl20-C11=1.747 H21-C12=1.084	C3-C2-C1=122.932 C4-C3-C2=117.402 C5-C4-C3=119.918 C6-C5-C4=121.701 C7-C1-C6=135.335 C8-C7-C1=105.107 C9-C8-C7=122.931 C10-C9-C8=117.394 C11-C10-C9=119.932 C12-C11-C10=121.693 O13-C8-C7 =112.091 Cl14-C3-C2=119.716 Cl15-C4-C3=119.587 Cl16-C5-C4=120.374 H17-C6-C5=119.8 Cl18-C9-C8=119.703 Cl19-C10-C9=119.566 Cl20-C11-C10=120.363 H21-Cl20-C11=119.681	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
20	C2-C1=1.408 C3-C2=1.389 C4-C3=1.394 C5-C4=1.403 C6-C5=1.392 C7-C1=1.452 C8-C7=1.405 C9-C8=1.384 C10-C9=1.396 C11-C10=1.413 C12-C11=1.394 O13-C8=1.370 Cl14-C3=1.743 H15-C4=1.083 Cl16-C5=1.757 H17-C6=1.084 H18-C9=1.083 Cl19-C10=1.745 Cl20-C11=1.748 H21-C12=1.0844	C3-C2-C1=121.965 C4-C3-C2=118.039 C5-C4-C3=119.880 C6-C5-C4=122.511 C7-C1-C6=135.011 C8-C7-C1=105.482 C9-C8-C7=123.348 C10-C9-C8=116.939 C11-C10-C9=120.992 C12-C11-C10=120.812 O13-C8-C7 =112.199 Cl14-C3-C2=120.924 H15-C4-C3=A119.842 Cl16-C5-C4=118.354 H17-C6-C5=120.646 H18-C9-C8=121.946 Cl19-C10-C9=117.994 Cl20-C11-C10=120.907 H21-Cl20-C11=119.494	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
21	C2-C1=1.410 C3-C2=1.389 C4-C3=1.394 C5-C4=1.403 C6-C5=1.393 C7-C1=1.453 C8-C7=1.406 C9-C8=1.383 C10-C9=1.394 C11-C10=1.414 C12-C11=B1.399 O13-C8=1.370 Cl14-C3=1.746 H15-C4=1.085 Cl16-C5=1.086 H17-C6=1.083 H18-C9=1.083 Cl19-C10=1.745 Cl20-C11=1.739 H21-C12=1.743	C3-C2-C1=122.449 C4-C3-C2=117.667 C5-C4-C3=120.544 C6-C5-C4=121.662 C7-C1-C6=136.011 C8-C7-C1=105.663 C9-C8-C7=123.937 C10-C9-C8=116.758 C11-C10-C9=121.745 C12-C11-C10=136.146 O13-C8-C7 =111.670 Cl14-C3-C2=120.763 H15-C4-C3=119.033 Cl16-C5-C4=118.772 H17-C6-C5=120.852 H18-C9-C8=121.948 Cl19-C10-C9=117.680 Cl20-C11-C10=120.193 H21-Cl20-C11=119.376	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=0.000
22	C2-C1=1.408 C3-C2=1.386 C4-C3=1.394	C3-C2-C1=123.946 C4-C3-C2=115.756 C5-C4-C3=122.390	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000

	C5-C4=1.403 C6-C5=1.392 C7-C1=1.452 C8-C7=1.407 C9-C8=1.383 C10-C9=1.394 C11-C10=1.413 C12-C11=1.399 O13-C8=1.371 Cl14-C3=1.083 H15-C4=1.755 Cl16-C5=1.084 H17-C6=1.083 H18-C9=1.083 Cl19-C10=1.745 Cl20-C11=1.739 H21-C12=1.743	C6-C5-C4=120.356 C7-C1-C6=136.410 C8-C7-C1=105.536 C9-C8-C7=123.849 C10-C9-C8=116.823 C11-C10-C9=121.740 C12-C11-C10=136.256 O13-C8-C7 =111.662 Cl14-C3-C2=122.019 H15-C4-C3=118.692 Cl16-C5-C4=119.330 H17-C6-C5=120.123 H18-C9-C8=121.952 Cl19-C10-C9=117.652 Cl20-C11-C10=120.239 H21-Cl20-C11=119.281	C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=0.000
23	C2-C1=1.406 C3-C2=1.383 C4-C3=1.396 C5-C4=1.412 C6-C5=1.394 C7-C1=1.450 C8-C7=1.409 C9-C8=1.392 C10-C9=1.402 C11-C10=1.403 C12-C11=1.390 O13-C8=1.367 Cl14-C3=1.083 H15-C4=1.744 Cl16-C5=1.747 H17-C6=1.083 H18-C9=1.733 Cl19-C10=1.743 Cl20-C11=1.083 H21-C12=1.749	C3-C2-C1=123.561 C4-C3-C2=116.888 C5-C4-C3=120.908 C6-C5-C4=120.989 C7-C1-C6=135.922 C8-C7-C1=105.279 C9-C8-C7=123.842 C10-C9-C8=116.374 C11-C10-C9=121.412 C12-C11-C10=120.512 O13-C8-C7 =111.812 Cl14-C3-C2=121.935 H15-C4-C3=117.989 Cl16-C5-C4=120.858 H17-C6-C5=119.705 H18-C9-C8=120.184 Cl19-C10-C9=120.505 Cl20-C11-C10=119.299 H21-Cl20-C11=119.392	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
24	C2-C1=1.410 C3-C2=1.385 C4-C3=1.395 C5-C4=1.402 C6-C5=1.392 C7-C1=1.450 C8-C7=1.405 C9-C8=1.389 C10-C9=1.405 C11-C10=1.414 C12-C11=1.392 O13-C8=1.369 Cl14-C3=1.083 H15-C4=1.752 Cl16-C5=1.083 H17-C6=1.750 H18-C9=1.734 Cl19-C10=1.735 Cl20-C11=1.747 H21-C12=1.0822	C3-C2-C1=124.421 C4-C3-C2=115.657 C5-C4-C3=122.619 C6-C5-C4=119.538 C7-C1-C6=136.910 C8-C7-C1=104.892 C9-C8-C7=123.028 C10-C9-C8=117.495 C11-C10-C9=119.797 C12-C11-C10=121.826 O13-C8-C7 =112.186 Cl14-C3-C2=122.097 H15-C4-C3=118.898 Cl16-C5-C4=120.278 H17-C6-C5=119.254 H18-C9-C8=119.624 Cl19-C10-C9=119.587 Cl20-C11-C10=120.327 H21-Cl20-C11=119.854	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
25	C2-C1=1.418 C3-C2=1.385 C4-C3=1.388 C5-C4=1.398 C6-C5=1.395 C7-C1=1.473 C8-C7=1.412 C9-C8=1.382	C3-C2-C1=126.368 C4-C3-C2=115.781 C5-C4-C3=121.477 C6-C5-C4=120.900 C7-C1-C6=140.587 C8-C7-C1=104.668 C9-C8-C7=125.618 C10-C9-C8=116.898	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000

	C10-C9=1.388 C11-C10=1.410 C12-C11=1.409 O13-C8=1.364 Cl14-C3=1.083 H15-C4=1.750 Cl16-C5=1.083 H17-C6=1.747 H18-C9=1.083 Cl19-C10=1.743 Cl20-C11=1.740 H21-C12=1.735	C11-C10-C9=120.868 C12-C11-C10=120.563 O13-C8-C7 =112.341 Cl14-C3-C2=121.393 H15-C4-C3=119.508 Cl16-C5-C4=119.880 H17-C6-C5=114.931 H18-C9-C8=121.367 Cl19-C10-C9=117.914 Cl20-C11-C10=119.202 H21-Cl20-C11=118.021	C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
26	C2-C1=1.406 C3-C2=1.387 C4-C3=1.394 C5-C4=1.405 C6-C5=1.392 C7-C1=1.451 C8-C7=1.405 C9-C8=1.310 C10-C9=1.406 C11-C10=1.414 C12-C11=1.392 O13-C8=1.369 Cl14-C3=1.083 Cl15-C4=1.755 H16-C5=1.084 H17-C6=1.086 Cl18-C9=1.735 Cl19-C10=1.736 Cl20-C11=1.748 H21-C12=1.084	C3-C2-C1=123.806 C4-C3-C2=115.668 C5-C4-C3=122.542 C6-C5-C4=120.189 C7-C1-C6=135.810 C8-C7-C1=105.151 C9-C8-C7=122.851 C10-C9-C8=117.583 C11-C10-C9=119.809 C12-C11-C10=121.703 O13-C8-C7 =112.101 Cl14-C3-C2=122.119 CL15-C4-C3=118.667 H16-C5-C4=119.290 H17-C6-C5=120.040 Cl18-C9-C8=119.629 Cl19-C10-C9=119.631 Cl20-C11-C10=120.384 H21-Cl20-C11=119.596	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 Cl14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
27	C2-C1=1.408 C3-C2=1.386 C4-C3=1.394 C5-C4=1.403 C6-C5=1.392 C7-C1=1.452 C8-C7=1.407 C9-C8=1.383 C10-C9=1.394 C11-C10=1.413 C12-C11=1.399 O13-C8=1.371 H14-C3=1.083 Cl15-C4=1.755 H16-C5=1.084 H17-C6=1.083 H18-C9=1.083 Cl19-C10=1.745 Cl20-C11=1.738 Cl21-C12=1.743	C3-C2-C1=123.929 C4-C3-C2=115.766 C5-C4-C3=122.388 C6-C5-C4=120.357 C7-C1-C6=136.392 C8-C7-C1=105.532 C9-C8-C7=123.856 C10-C9-C8=116.825 C11-C10-C9=121.740 C12-C11-C10=136.280 O13-C8-C7 =111.666 H14-C3-C2=122.002 Cl15-C4-C3=118.696 H16-C5-C4=119.330 H17-C6-C5=120.154 H18-C9-C8=121.961 Cl19-C10-C9=117.653 Cl20-C11-C10=120.231 Cl21-Cl20-C11=119.254	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=0.000
28	C2-C1=1.406 C3-C2=1.383 C4-C3=1.396 C5-C4=1.412 C6-C5=1.394 C7-C1=1.450 C8-C7=1.409 C9-C8=1.392 C10-C9=1.402 C11-C10=1.403 C12-C11=1.390 O13-C8=1.367 H14-C3=1.083	C3-C2-C1=123.561 C4-C3-C2=116.888 C5-C4-C3=120.908 C6-C5-C4=120.989 C7-C1-C6=135.922 C8-C7-C1=105.279 C9-C8-C7=123.842 C10-C9-C8=116.374 C11-C10-C9=121.412 C12-C11-C10=120.512 O13-C8-C7 =111.812 H14-C3-C2=121.935 Cl15-C4-C3=117.989	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000

	Cl15-C4=1.744 Cl16-C5=1.747 H17-C6=1.083 Cl18-C9=1.733 Cl19-C10=1.743 H20-C11=1.083 Cl21-C12=1.749	Cl16-C5-C4=120.858 H17-C6-C5=119.705 Cl18-C9-C8=120.184 Cl19-C10-C9=120.505 H20-C11-C10=119.299 Cl21-H20-C11=119.393	H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 H20-C11-C10-C9=180.000 Cl21-H20-C11-C10=180.000
29	C2-C1=1.410 C3-C2=1.385 C4-C3=1.395 C5-C4=1.402 C6-C5=1.392 C7-C1=1.450 C8-C7=1.405 C9-C8=1.389 C10-C9=1.405 C11-C10=1.414 C12-C11=1.392 O13-C8=1.369 H14-C3=1.083 Cl15-C4=1.752 H16-C5=1.083 Cl17-C6=1.750 Cl18-C9=1.734 Cl19-C10=1.735 Cl20-C11=1.747 H21-C12=1.082	C3-C2-C1=124.421 C4-C3-C2=115.657 C5-C4-C3=122.619 C6-C5-C4=119.538 C7-C1-C6=136.910 C8-C7-C1=104.892 C9-C8-C7=123.028 C10-C9-C8=117.495 C11-C10-C9=119.797 C12-C11-C10=121.826 O13-C8-C7 =112.186 H14-C3-C2=122.097 Cl15-C4-C3=118.898 H16-C5-C4=120.278 Cl17-C6-C5=119.254 Cl18-C9-C8=119.624 Cl19-C10-C9=119.587 Cl20-C11-C10=120.327 H21-Cl20-C11=119.854	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 H16-C5-C4-C3=180.000 Cl17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 H21-Cl20-C11-C10=180.000
30	C2-C1=1.407 C3-C2=1.384 C4-C3=1.396 C5-C4=1.412 C6-C5=1.394 C7-C1=1.451 C8-C7=1.407 C9-C8=1.383 C10-C9=1.394 C11-C10=1.414 C12-C11=1.399 O13-C8=1.371 H14-C3=1.083 Cl15-C4=1.744 Cl16-C5=1.747 H17-C6=1.082 H18-C9=1.083 Cl19-C10=1.744 Cl20-C11=1.738 Cl21-C12=1.742	C3-C2-C1=123.507 C4-C3-C2=116.983 C5-C4-C3=120.870 C6-C5-C4=120.975 C7-C1-C6=136.121 C8-C7-C1=105.437 C9-C8-C7=123.798 C10-C9-C8=116.804 C11-C10-C9=121.778 C12-C11-C10=136.242 O13-C8-C7 =111.720 H14-C3-C2=121.885 Cl15-C4-C3=118.002 Cl16-C5-C4=120.844 H17-C6-C5=119.667 H18-C9-C8=121.972 Cl19-C10-C9=117.637 Cl20-C11-C10=120.253 Cl21-Cl20-C11=119.286	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =0.000 H14-C3-C2-C1=180.000 Cl15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 H18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=0.000
31=64	C2-C1=1.408 C3-C2=1.390 C4-C3=1.393 C5-C4=1.403 C6-C5=1.400 C7-C1=1.454 C8-C7=1.408 C9-C8=1.390 C10-C9=1.391 C11-C10=1.404 C12-C11=1.400 O13-C8=1.370 Cl14-C3=1.742 H15-C4=1.083 Cl16-C5=1.756 H17-C6=1.082 Cl18-C9=1.740 H19-C10=1.083	C3-C2-C1=122.298 C4-C3-C2=117.874 C5-C4-C3=119.856 C6-C5-C4=119.903 C7-C1-C6=135.318 C8-C7-C1=105.180 C9-C8-C7=122.611 C10-C9-C8=117.603 C11-C10-C9=120.892 C12-C11-C10=121.217 O13-C8-C7 =112.190 Cl14-C3-C2=120.977 H15-C4-C3=119.864 Cl16-C5-C4=118.259 H17-C6-C5=121.781 Cl18-C9-C8=121.074 H19-C10-C9=119.774 Cl20-C11-C10=117.760	C4-C3-C2-C1=0.000 C5-C4-C3-C2=0.000 C6-C5-C4-C3=0.000 C7-C1-C6-C5=180.000 C8-C7-C1-C6=180.000 C9-C8-C7-C1=180.000 C10-C9-C8-C7=0.000 C11-C10-C9-C8=0.000 C12-C11-C10-C9=0.000 O13-C8-C7-C1 =180.000 Cl14-C3-C2-C1=180.000 H15-C4-C3-C2=180.000 Cl16-C5-C4-C3=180.000 H17-C6-C5-C4=180.000 Cl18-C9-C8-C7=180.000 Cl19-C10-C9-C8=180.000 Cl20-C11-C10-C9=180.000 Cl21-Cl20-C11-C10=180.000

	Cl20-C11=1.746 Cl21-C12=1.741	Cl21-Cl20-C11=121.553	

Table 2: Energy (au), Hardness (eV), Chemical Potential (eV), Electrophilicity (eV) and Local Electrophilicities (eV) (MPA and HPA) for Different Polychlorinated Dibenzofurans.

Molecule	Energy (a.u.)	η (eV)	μ (eV)	ω (eV)	ω^{+}_{Max} (eV) MPA	ω^{+}_{Max} (eV) HPA
1	-996.924	2.493	-3.712	2.763	0.429	0.224
2	-996.922	2.528	-3.694	2.699	0.430	0.251
3	-1456.516	2.452	-3.999	3.101	0.466	0.273
4	-1456.518	2.453	-3.950	3.180	0.466	0.248
5	-1916.110	2.451	-4.062	3.366	0.511	0.343
6	-1916.112	2.399	-4.054	3.425	0.512	0.346
7	-1916.100	2.439	-4.031	3.331	0.530	0.326
8	-1916.108	2.414	-4.103	3.486	0.538	0.345
9	-2375.691	2.412	-4.201	3.659	0.565	0.351
10	-2375.694	2.392	-4.234	3.748	0.570	0.360
11	-2375.702	2.400	-4.253	3.769	0.569	0.373
12	-2375.697	2.347	-4.215	3.785	0.548	0.360
13	-2375.698	2.363	-4.202	3.736	0.599	0.329
14	-2835.285	2.403	-4.358	3.952	0.611	0.375
15	-2835.282	2.340	-4.309	3.967	0.617	0.377
16	-2835.285	2.329	-4.319	4.005	0.579	0.376
17	-2835.283	2.343	-4.354	4.046	0.586	0.376
18	-3294.871	2.309	-4.437	4.263	0.638	0.388
19	-3294.868	2.342	-4.485	4.293	0.603	0.386
20	-2375.698	2.402	-4.288	3.828	0.566	0.367
21	-2375.694	2.414	-4.193	3.642	0.571	0.357
22	-2375.697	2.356	-4.151	3.657	0.559	0.351
23	-2835.288	2.325	-4.307	3.989	0.586	0.379
24	-2835.287	2.349	-4.328	3.988	0.591	0.379
25	-2835.278	2.330	-4.323	4.010	0.579	0.377
26	-2375.694	2.366	-4.179	3.691	0.556	0.354
27	-2375.697	2.356	-4.151	3.657	0.558	0.351
28	-2835.288	2.325	-4.307	3.989	0.586	0.379
29	-2835.287	2.349	-4.328	3.988	0.591	0.379
30	-2835.285	2.329	-4.319	4.005	0.579	0.376
31	-2835.288	2.338	-4.361	4.067	0.633	0.342

Table 3: Hardness (eV), Chemical Potential (eV), Electrophilicity (eV) of Nucleic Acid Bases/DNA Base Pairs.

Moleule	η (eV)	μ (eV)	ω eV
Adenine	2.850	-3.103	1.689
Thymine	2.894	-3.689	2.351
Guanine	2.916	-2.648	1.202
Cytosine	2.785	-3.370	2.039
Uracil	2.962	-3.919	2.593
GCWC	2.018	-3.030	2.275
ATH	2.526	-3.256	2.099