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Abstract

Owing to its successful application to complex molecular systems, computational density functional theory (DFT) has been used to study the effect of an electric field on the molecular polarizability and HOMO–LUMO gap of 1-phenyl-4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}benzene (1) and its fluoro-, chloro-, and cyano- derivatives, namely, 1-fluoro-4-(4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenyl)benzene (2), 1-chloro-4-(4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenyl)benzene (3), and 4-(4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenyl)benzonitrile (4). These molecules belong to the family of nematic liquid crystals with three rings: two benzene and one cyclohexane. Furthermore, two DFT approaches, namely, B3LYP and M062X, have been used to examine the results obtained. This study reveals a remarkable feature: the polarizability of these molecules follows nearly a step function when varied with respect to the electric field. The 4-(4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenyl)benzonitrile (4) polarizes more than all other derivatives, whereas 1-fluoro-4-(4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenyl)benzene (2) has the widest stability region of them all. With the increase in the electric field, polarizability increases in a smooth manner until a point called here the shoot-up point at which polarizability switches to a higher value and remains nearly constant as the field increases further. However, beyond a certain value of the electric field, polarizability undergoes a steep fall. It is also found that the effective length (long molecular axis) of the molecule has a direct effect on its polarizability.

Keywords: polarizability, liquid crystal, nematic, density functional theory

Introduction

“Liquid crystal” or “mesophase” are the terms used to describe a state of matter that exhibits mechanical and symmetric properties between those of a viscous liquid and a crystal. Nematic liquid crystals consist of rod-like molecules that, on an average, line up parallel to a preferred direction. This orientation of molecules is modified when placed in an electric or magnetic field [1, 2]. Research on liquid crystals is an ever-evolving field, with several novel and high-end applications of these molecules, but there is always scope to improve and enhance their performance. Novel molecules that are promising candidates for liquid crystal applications are a vital area of research. With the assistance of state-of-the-art computational techniques, this research can be helpful in understanding the nature and properties of mesophase molecules.

The dielectric constants of liquid crystals are anisotropic. The relationship between the dielectric constant

and molecular polarizability of liquid crystals can be described by the Maier–Meier equations [3]. Interactions between molecules and forces like dispersion are affected by polarizability and polarization caused by external and internal factors [4].

The effect of an electric field on liquid crystal molecules is an important area of investigation as most liquid crystal devices use electric fields, optical fields, or thermally induced refractive index changes to modulate light [5]. Upadhyay *et al.* [6] reported the effect of continually increasing the electric field on the polarizability of 5CB and its derivatives, which are room-temperature nematics with two benzene rings without any linker. Using a molecular dynamics simulation, coarse-grained dynamics simulation, and density functional theory (DFT), Ju *et al.* [7] have worked on 5CB to predict some of its physical properties. Similarly, Kumar *et al.* [8] used DFT method for investigating odd–even effects under the influence of an external applied electric field on N(p-n-heptyloxy-benzylidene)p-toluidine by increasing

Table 1. List of Molecules Studied with their Transition Temperatures (°C), Birefringence (20°C) and Dielectric Anisotropy (Extrapolated to 100% at 20 °C) (Ref. [9])

Compound	Molecular Structure	Transition Temperature (°C)			Δn	$\Delta\epsilon^a$	References
		Crystal	Nematic	Smectic A			
1		67	82	-	0.15	≈ 0	[10]
2		76	125	-	0.17	+4.9	[10]
3		100	158	-	0.22	+7.5	[10]
4		79	87	184	0.23	+13	[11]

the length of an alkyl chain. Therefore, taking a hint from these studies in general and from Upadhyay *et al.* [6] in particular, it seems necessary to study effects on a different set of molecules, where the number of rings is greater than two so that it can be determined that previously observed effects apply to other nematics too.

This paper presents a comparative study of the effect of a continually increasing electric field on the molecular polarizability and HOMO–LUMO gap of 1-phenyl-4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}benzene (1) and its fluoro-, chloro-, and cyano- derivatives: 1-fluoro-4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenylbenzene (2), 1-chloro-4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenylbenzene (3), and 4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}phenylbenzonitrile (4), respectively. They are all nematic liquid crystals consisting of two benzene rings linked to a third cyclohexane ring with an ethyl linker in between. They have positive dielectric anisotropy and effective lengths (long molecular axis) of 21 to 22 Å. Table 1 gives a summary of the molecular structure, transition temperatures, and dielectric contents of the molecules studied.

Methods

The molecules under study were designed using Gauss View 5.0 and the structures of these molecules were optimized using computational DFT, which has delivered several promising results for characterization, explanation, and establishing a correlation of properties of various types of molecules [12, 13]. Structural optimization

and energy calculations were performed using the B3LYP [14, 15] hybrid functional for Gaussian-type orbitals and the 6-31G** [16] basis set in the Gaussian 09 package [17]. The dihedral angle of the linker between cyclohexane and the benzene ring was varied from 0° to 350° to find the minimum energy configuration of the structures. The variation of molecular polarizability (α) on application of the electric field was calculated using the B3LYP and M062X [18] methods using a 6-31G** basis set with the help of the Gaussian 09 package.

Jensen [19] explained the calculation of polarizability as implemented in Gaussian 09. Starting with an initial value of 0.000 a.u., the field was varied through increments of 0.002 a.u. The trace of the polarizability tensor, thus, obtained was used to find the value of polarizability.

Results

A dihedral angle of 180° for the linker yields the minimum energy for the molecular structures of all compounds. The next two minimum energy points are 70° and 290°. The fluctuation of energy with a dihedral angle is provided in Supporting Information Figures S1, S2, S3, and S4. Figure 1 presents the optimized geometries of molecules 1, 2, 3, and 4 at dihedral angles around 180°.

Linker dihedral angles and inter-ring distances after optimization are given in Table 2.

Figure S1. Energy Fluctuation with the Change in the Dihedral Angle from 0° to 350° for Compound 1, 1-phenyl-4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}benzene. The Minimum Energy is at 180° and Next Two Minima are at 70° and 290°

Figure S3. Energy Fluctuation with the Change in the Dihedral Angle from 0° to 350° for Compound 3, 1-chloro-4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzene. Minimum Energy is at 180° and the Next Two Minima are at 70° and 290°

Figure S2. Energy Fluctuation with the Change in the Dihedral Angle from 0° to 350° for Compound 2, 1-fluoro-4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzene. Minimum Energy is at 180° and the Next Two Minima are at 70° and 290°

Figure S4. Energy Fluctuation with the Change in the Dihedral Angle from 0° to 350° for Compound 4, 4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzonitrile. Minimum Energy is at 180° and the Next Two Minima are at 70° and 290°

Figure 1. Optimized geometries for molecules (a) 1-phenyl-4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}benzene (long molecular length = 21.263 Å) and its fluoro-, chloro-, and cyano- derivatives (b) 1-fluoro-4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzene (long molecular length = 21.445 Å), (c) 1-chloro-4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzene (long molecular length = 21.899 Å), (d) 4-{4-[2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl]phenyl}benzonitrile (long molecular length = 22.726 Å)

Table 2. Linker Dihedral and Inter-ring Distances of Compounds

Compound	Linker Dihedral (°)	Inter-ring Distance (Å)
1	-178.821	1.485
2	176.808	1.484
3	178.863	1.484
4	177.067	1.482

Figure 2. (a) Variation of Polarizability with Electric Field and (b) Variation of HOMO–LUMO gap for Molecule 1

1-phenyl-4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}benzene. With no electric field, molecule 1 shows polarizability around 272.6 a.u. for B3LYP and 270.1 a.u. for M062X. It increases slowly until the electric field is 0.012 a.u. for B3LYP and 0.016 for M062X. Beyond this, polarizability increases sharply (here called the shoot-up point) to approximately 1316 and 1650 a.u. for B3LYP and M062X, respectively. Polarizability remains stable up to an electric field of 0.034 a.u. for B3LYP and 0.032 a.u. for M062X and exhibits a sharp decrease thereafter (Figure 2). The HOMO–LUMO gap also varies with the electric field, as shown in Figure 2. It can be seen that the HOMO–LUMO gap achieves stabilization for the same value at which there is the stabilization of polarizability.

1-fluoro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene. Substituting hydrogen with fluorine in the benzene ring at one end of the molecule (Figure 1(b)) resulted in increased long molecular length (as shown in Figure 1), which in turn raised the zero-field polarizability by a small amount (approximately 273.2 and 270.5 a.u. for B3LYP and M062X, respectively). Polarizability sharply increases beyond an electric field of 0.018 a.u. and 0.022 a.u. for B3LYP and M062X (increments of 0.06 a.u. for each), respectively, up to polarizabilities of approximately 1324 and 1691 a.u.,

respectively. After remaining stable between electric fields of 0.020–0.046 a.u. for B3LYP and 0.024–0.046 a.u. for M062X, polarizability steeply falls. The variation in the HOMO–LUMO gap is modified in accordance with the electric field, as shown in Figure 3.

1-chloro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene. When fluorine is replaced with another halogen chlorine, this results in a slight increase in effective length (long molecular axis) and higher zero-field polarizability (approximately 289 and 285 a.u. for B3LYP and M062, respectively) than the previous two cases. Although the shoot-up point for the electric field has been reduced by 0.04 a.u. (0.016 and 0.02 a.u., respectively), the stability region has narrowed by 0.06 a.u. for both B3LYP and M062X. The electric field values at which a sharp decrease occurs are 0.036 a.u. and 0.034 a.u. for B3LYP and M062X, respectively. Here, the HOMO–LUMO gap and molecular polarizability also become stabilized for the same set of electric field values.

4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzonitrile. Replacement by a cyano- group produces not only the longest effective length (long molecular length) but also the highest zero-field polarizability (approximately 298 and 293 a.u. for B3LYP and M062X,

Figure 3. (a) Variation of Polarizability with Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 2

Figure 4. (a) Variation of Polarizability with Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 3

Figure 5. (a) Variation of Polarizability with Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 4

respectively) of all cases. The shoot-up point (0.018 and 0.022 a.u., respectively) is 0.02 a.u. higher than that in the previous case and the point where a steep decrease begins is 0.04 and 0.034 a.u. for B3LYP and M062X, respectively. The polarizability in the stability region is highest (approximately 1492 and 1879 a.u. for B3LYP and M062X, respectively) among the previous cases. The corresponding HOMO–LUMO gap variation is shown in Figure 5.

Effect of the field on the charge distribution. The conjugation effect that arises because of the increasing electric field can be justified by the Mulliken charge distribution on the respective atoms of these molecules at three electric fields, which correspond to the initial lower value of polarizability (before the shoot-up point), region of stability, and region in which polarizability drops. The Mulliken charge values are provided in Tables S1 to S12 (Supporting Information).

Discussion

To ascertain the results obtained using the B3LYP exchange-correlation functional, it was decided to use another exchange-correlation functional, M062X. Since

the study is based on theoretical calculations, it is important to validate the results obtained from one functional with those from another. Moreover, both functionals have a proven track record when applied to DFT calculations in complex molecules [18, 20].

The patterns of variation of polarizability and of the HOMO–LUMO gap were found to be similar to those obtained by Upadhyay *et al.* [6] for two-ringed 5CB (along with its derivatives) but with greater sharpness at the points of abrupt change. The variations in the HOMO–LUMO gap and the polarizability with electric field have a common feature, i.e., there are two regions, upper and lower, in which polarizability remains almost stable with a shoot-up point between these two regions. The HOMO–LUMO gap decreases in a uniform manner and then becomes stabilized. Compound **4** is polarized most compared with the others, whereas compound **2** has the widest upper stability region. The shoot-up point is the lowest for compound **1**. Above this point, polarizability increases because, owing to the conjugation effect, which increases the number of mobile electrons, hydrogen atoms attached to the end carbon atoms of the alkyl chain start gaining negative charge, as can be seen in Figure 6. As the field is gradually increases, the polarizability achieves

Figure 6. Variation of Mulliken Charge Distribution on the Hydrogen Atom Attached to the end Carbon Atom of the Alkyl Chain of all Four Molecules. In Each Case, it Gains a Negative Charge Beyond the Shoot-up Point

stability owing to the availability of a large number of mobile electrons, which cause a near saturation of mobile charge carriers). Furthermore, the availability of mobile electrons due to conjugation decreases HOMO–LUMO separation. Polarizability undergoes a steep fall beyond a certain value of the electric field as a result of random distribution of negative charges caused by a sufficiently high electric field.

Except for compound **1**, all compounds have an electronegative functional group at one end. Compound **2**, despite having the most electronegative atom, fluorine, at one end, becomes the least polarized (compared with compounds **3** and **4**) in the electric field instability region and it is only slightly more polarized than compound **1**. The effective length (long molecular axis) of the molecule has a direct effect on its polarizability. As seen from Figure 1, the molecule with a larger length has greater polarizability than the others, but also molecule **2** has the widest stability region.

On application of the electric field, both M062X and B3LYP start with nearly identical values of polarizability (slightly higher for B3LYP), but in the upper stability region, M062X gives a much higher value than B3LYP. In addition, the shoot-up point for M062X is higher than that for B3LYP. The upper stability region is wider for B3LYP than M062X. Moreover, the HOMO–LUMO gap is flat in the stability region of the respective molecules.

Conclusion

These compounds (1-phenyl-4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl] ethyl}benzene (**1**) and its fluoro-, chloro-, and cyano- derivatives, namely, 1-fluoro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene (**2**), 1-chloro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene (**3**), and 4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl) benzonitrile (**4**).) are used in numerous applications such as LCDs and Spatial Light Modulators. Therefore, it is important to understand how electric fields affect liquid crystal molecules in terms of polarizability, as this is a deciding factor for dispersion forces and interaction energy in a bulk material. The study of polarizability is also important for electro-optic properties such as birefringence and the dielectric constant. The above studies showed that there is a certain range of applied electric fields for which polarizability and the HOMO–LUMO gap remain stable

or constant. This study revealed a remarkable feature, namely, that the polarizability of these molecules follows nearly a step function. This can be attributed to the charge conjugation effect that comes into play as the magnitude of the electric field is increased. However, as the strength of the electric field crosses a certain high value, the availability of a large number of charge carriers causes a sudden drop in the polarizability, which is expected because a large number of mobile charge carriers makes the molecule less polarizable. The substitution of hydrogen with different groups, such as fluorine, chlorine, and cyano- affects the molecular length as well as the charge distribution, which has a direct effect on the magnitude of polarizability.

As no experimental data are available for these molecules and for such study, it cannot be determined precisely which model is closer to reality. M062X is accurate in predicting valence and Rydberg electronic excitation energies, including dispersion corrections and provides excellent results for aromatic–aromatic stacking interactions [6]. M06 functionals perform better than B3LYP for a model system with dispersion and ionic hydrogen-bonding interactions [20], whereas spectroscopic studies show that the B3LYP method is a better predictor of the experimental values than the M062X method [21].

However, this study established how the polarizability and HOMO–LUMO gap for these molecules vary with an externally applied electric field. Although the values obtained using the B3LYP and M062X functionals are different, the trends followed by both the polarizability and the HOMO–LUMO gap are similar in both cases. Therefore, this study established how the polarizability and the HOMO–LUMO gap of these molecules will vary with the intensity of the externally applied electric field.

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Appendices

Figure S5. Optimized Geometries for Molecules (a) 1-phenyl-4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}benzene and its fluoro-, chloro- and cyano- derivatives (b) 1-fluoro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene, (c) 1-chloro-4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzene, and (d) 4-(4-{2-[(1*s*,4*r*)-4-pentylcyclohexyl]ethyl}phenyl)benzonitrile at Approximately 70°

Figure S6. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 1 Around 70°

Figure S7. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 2 Around 70°

Figure S8. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 3 Around 70°

Figure S9. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 4 Around 70°

Figure S10. Optimized Geometries for Molecules (a) 1-phenyl-4-{2-[(1s,4r)-4-pentylcyclohexyl]ethyl}benzene and its fluoro-, chloro-, and cyano- derivatives (b) 1-fluoro-4-{4-[2-[(1s,4r)-4-pentylcyclohexyl]ethyl]phenyl}benzene, (c) 1-chloro-4-{4-[2-[(1s,4r)-4-pentylcyclohexyl]ethyl]phenyl}benzene, and (d) 4-{4-[2-[(1s,4r)-4-pentylcyclohexyl]ethyl]phenyl}benzonitrile at Approximately 290° .

Figure S11. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 1 approximately 290°

Figure S12. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO-LUMO gap for Molecule 2 approximately 290°

Figure S13. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO–LUMO gap for Molecule 3 approximately 290°

Figure S14. (a) Variation of Polarizability with the Electric Field and (b) Variation of HOMO–LUMO gap for Molecule 4 approximately 290°

Table S1. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure 1) of Molecule 1 (Dihedral Angle around 70°)

MOLECULE 1					
B3LYP			M062X		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
1 C -0.088809	1 C -0.076524	1 C 0.026593	1 C -0.124064	1 C -0.120907	1 C -0.001726
2 C -0.115019	2 C -0.106203	2 C -0.060541	2 C -0.136565	2 C -0.137079	2 C -0.089678
3 C 0.058489	3 C 0.071372	3 C 0.152385	3 C 0.031872	3 C 0.030617	3 C 0.136470
4 C -0.113888	4 C -0.104926	4 C -0.051122	4 C -0.135380	4 C -0.134749	4 C -0.073640
5 C -0.088295	5 C -0.078769	5 C -0.025643	5 C -0.124092	5 C -0.122561	5 C -0.070047
6 H 0.149846	6 H 0.202813	6 H 0.393120	6 H 0.185504	6 H 0.215944	6 H 0.425942
7 H 0.102212	7 H 0.132689	7 H 0.262335	7 H 0.134613	7 H 0.143042	7 H 0.298142
8 H 0.041020	8 H 0.045962	8 H 0.125773	8 H 0.072499	8 H 0.049036	8 H 0.163974
9 H 0.095645	9 H 0.127428	9 H 0.271999	9 H 0.131117	9 H 0.136891	9 H 0.309486
10 C 0.062538	10 C 0.061514	10 C 0.056297	10 C 0.034301	10 C 0.035310	10 C 0.012230
11 C -0.108575	11 C -0.100781	11 C -0.060705	11 C -0.126928	11 C -0.123556	11 C -0.078864
12 C -0.109254	12 C -0.101744	12 C -0.055915	12 C -0.127349	12 C -0.125438	12 C -0.072903
13 C -0.136549	13 C -0.136566	13 C -0.125951	13 C -0.159200	13 C -0.163369	13 C -0.153312
14 H 0.108825	14 H 0.127874	14 H 0.203525	14 H 0.143594	14 H 0.155501	14 H 0.234113
15 C -0.143909	15 C -0.142689	15 C -0.129192	15 C -0.168313	15 C -0.170767	15 C -0.158174
16 H 0.106381	16 H 0.125782	16 H 0.207480	16 H 0.141463	16 H 0.152303	16 H 0.238605
17 C 0.125435	17 C 0.126533	17 C 0.147242	17 C 0.080509	17 C 0.075636	17 C 0.099918
18 H 0.052627	18 H 0.054136	18 H 0.094063	18 H 0.085824	18 H 0.071911	18 H 0.123558
19 H 0.056328	19 H 0.061631	19 H 0.115438	19 H 0.090863	19 H 0.079701	19 H 0.146636
20 C -0.243333	20 C -0.244576	20 C -0.251789	20 C -0.269125	20 C -0.268803	20 C -0.278046

Table S1. Continue

MOLECULE 1						
B3LYP			M062X			
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	
21 C -0.161296	21 C -0.160653	21 C -0.165689	21 C -0.193836	21 C -0.189760	21 C -0.196811	
22 C -0.040273	22 C -0.038693	22 C -0.034332	22 C -0.078493	22 C -0.076657	22 C -0.072691	
23 C -0.176526	23 C -0.177322	23 C -0.180348	23 C -0.205878	23 C -0.207181	23 C -0.210278	
24 C -0.168473	24 C -0.164770	24 C -0.153292	24 C -0.201441	24 C -0.196799	24 C -0.184186	
25 H 0.064844	25 H 0.064301	25 H 0.066657	25 H 0.083525	25 H 0.081181	25 H 0.085214	
26 C -0.185173	26 C -0.187211	26 C -0.188569	26 C -0.218795	26 C -0.223143	26 C -0.223479	
27 H 0.092640	27 H 0.095495	27 H 0.097927	27 H 0.110182	27 H 0.116427	27 H 0.115109	
28 H 0.151640	28 H 0.163948	28 H 0.176281	28 H 0.171136	28 H 0.196890	28 H 0.199456	
29 C -0.163610	29 C -0.157255	29 C -0.131436	29 C -0.196512	29 C -0.189797	29 C -0.163346	
30 H 0.078551	30 H 0.075332	30 H 0.061693	30 H 0.096228	30 H 0.094245	30 H 0.078677	
31 H 0.053765	31 H 0.039588	31 H -0.010683	31 H 0.077216	31 H 0.063181	31 H 0.011259	
32 C -0.048735	32 C -0.047863	32 C -0.041667	32 C -0.087646	32 C -0.087520	32 C -0.079286	
33 H 0.104209	33 H 0.112382	33 H 0.133112	33 H 0.129859	33 H 0.140480	33 H 0.159300	
34 H 0.080646	34 H 0.082179	34 H 0.088118	34 H 0.098109	34 H 0.098774	34 H 0.106261	
35 H 0.092743	35 H 0.003846	35 H -0.057235	35 H 0.047475	35 H 0.015438	35 H -0.040118	
36 H 0.065200	36 H 0.059438	36 H 0.042946	36 H 0.082657	36 H 0.074792	36 H 0.061051	
37 H 0.073379	37 H 0.070580	37 H 0.052494	37 H 0.092622	37 H 0.093772	37 H 0.070589	
38 C -0.165419	38 C -0.161997	38 C -0.139364	38 C -0.199312	38 C -0.200860	38 C -0.171691	
39 H 0.100290	39 H 0.106304	39 H 0.113178	39 H 0.121318	39 H 0.131586	39 H 0.135629	
40 H 0.077400	40 H 0.075493	40 H 0.068750	40 H 0.092848	40 H 0.089141	40 H 0.086652	
41 C -0.168384	41 C -0.162333	41 C -0.116706	41 C -0.206782	41 C -0.202193	41 C -0.165580	
42 H 0.059726	42 H 0.037992	42 H -0.084385	42 H 0.075890	42 H 0.060796	42 H -0.051168	
43 H 0.085138	43 H 0.072068	43 H -0.022336	43 H 0.108297	43 H 0.109475	43 H 0.008522	
44 C -0.159390	44 C -0.131299	44 C 0.042158	44 C -0.199302	44 C -0.195004	44 C -0.000883	
45 H 0.105425	45 H 0.095558	45 H 0.018509	45 H 0.125371	45 H 0.136318	45 H 0.043011	
46 H 0.029271	46 H -0.033117	46 H -0.372773	46 H 0.049793	46 H 0.021121	46 H -0.355134	
47 C -0.158056	47 C -0.124600	47 C 0.025178	47 C -0.206361	47 C -0.201260	47 C 0.002961	
48 H 0.133561	48 H 0.122363	48 H 0.041485	48 H 0.154045	48 H 0.174154	48 H 0.055680	
49 H 0.057293	49 H -0.010754	49 H -0.383998	49 H 0.077152	49 H 0.061253	49 H -0.380220	
50 C -0.307840	50 C -0.211951	50 C 0.250912	50 C -0.353066	50 C -0.349413	50 C 0.213098	
51 H 0.071332	51 H -0.024724	51 H -0.526313	51 H 0.092260	51 H 0.078610	51 H -0.529904	
52 H 0.119988	52 H 0.070588	52 H -0.179038	52 H 0.138217	52 H 0.148556	52 H -0.166786	
53 H 0.043669	53 H -0.103675	53 H -0.759809	53 H 0.059269	53 H 0.029067	53 H -0.749786	
54 C -0.074085	54 C -0.046894	54 C 0.154245	54 C -0.109420	54 C -0.102326	54 C 0.161840	
55 H 0.149051	55 H 0.206292	55 H 0.408007	55 H 0.184773	55 H 0.215343	55 H 0.443689	
56 H 0.078672	56 H 0.079494	56 H 0.099902	56 H 0.099819	56 H 0.093202	56 H 0.119484	
57 H 0.120432	57 H 0.132914	57 H 0.186481	57 H 0.147695	57 H 0.155000	57 H 0.212536	
58 H 0.050342	58 H 0.040213	58 H 0.024569	58 H 0.072232	58 H 0.054295	58 H 0.043255	
59 H 0.091837	59 H 0.093785	59 H 0.099979	59 H 0.107718	59 H 0.110150	59 H 0.115391	

Table S2. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure 1) of Molecule 2 (Dihedral Angle around 70°)

MOLECULE 2					
B3LYP			B3LYP		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
1 C -0.147998	1 C -0.129804	1 C -0.029906	1 C -0.179548	1 C -0.175722	1 C -0.054444
2 C -0.110845	2 C -0.103058	2 C -0.065969	2 C -0.131058	2 C -0.131602	2 C -0.090616
3 C 0.054132	3 C 0.067902	3 C 0.151344	3 C 0.026707	3 C 0.025294	3 C 0.136766
4 C -0.111416	4 C -0.104165	4 C -0.071232	4 C -0.131782	4 C -0.132471	4 C -0.095670
5 C -0.146939	5 C -0.129207	5 C -0.038135	5 C -0.178445	5 C -0.174685	5 C -0.066269
6 C 0.407960	6 C 0.437897	6 C 0.578623	6 C 0.415186	6 C 0.426595	6 C 0.609919
7 H 0.146120	7 H 0.191729	7 H 0.354510	7 H 0.184344	7 H 0.204987	7 H 0.390656
8 H 0.099266	8 H 0.125695	8 H 0.238072	8 H 0.132619	8 H 0.134783	8 H 0.275566
9 H 0.068002	9 H 0.081893	9 H 0.166008	9 H 0.101002	9 H 0.087116	9 H 0.205154
10 H 0.124680	10 H 0.162084	10 H 0.308127	10 H 0.162921	10 H 0.173756	10 H 0.346485
11 C 0.063187	11 C 0.062081	11 C 0.058523	11 C 0.034726	11 C 0.035862	11 C 0.014027
12 C -0.110328	12 C -0.101918	12 C -0.053503	12 C -0.128470	12 C -0.124877	12 C -0.067230
13 C -0.109963	13 C -0.102722	13 C -0.064979	13 C -0.128513	13 C -0.126795	13 C -0.082506
14 C -0.138578	14 C -0.138743	14 C -0.126387	14 C -0.161934	14 C -0.167537	14 C -0.154442
15 H 0.127995	15 H 0.155847	15 H 0.254937	15 H 0.162941	15 H 0.183891	15 H 0.286655
16 C -0.142871	16 C -0.140044	16 C -0.123129	16 C -0.164230	16 C -0.164900	16 C -0.149104
17 H 0.080315	17 H 0.089023	17 H 0.139922	17 H 0.115150	17 H 0.113272	17 H 0.172102
18 C 0.130256	18 C 0.132495	18 C 0.153702	18 C 0.086391	18 C 0.082562	18 C 0.108032
19 H 0.081868	19 H 0.097210	19 H 0.171602	19 H 0.115626	19 H 0.116389	19 H 0.203501
20 H 0.036640	20 H 0.034173	20 H 0.063019	20 H 0.069180	20 H 0.046596	20 H 0.092419

Table S2. *Continue*

MOLECULE 2					
B3LYP			B3LYP		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
21 C -0.245047	21 C -0.247293	21 C -0.256852	21 C -0.271986	21 C -0.272260	21 C -0.284085
22 C -0.171907	22 C -0.173023	22 C -0.182704	22 C -0.203786	22 C -0.201653	22 C -0.215153
23 C -0.037605	23 C -0.035462	23 C -0.030387	23 C -0.075971	23 C -0.072132	23 C -0.067026
24 C -0.171118	24 C -0.168981	24 C -0.162360	24 C -0.202848	24 C -0.200376	24 C -0.194145
25 C -0.177542	25 C -0.178940	25 C -0.183650	25 C -0.207901	25 C -0.210130	25 C -0.214970
26 H 0.039785	26 H 0.028804	26 H 0.003816	26 H 0.058961	26 H 0.041027	26 H 0.020398
27 C -0.167214	27 C -0.162513	27 C -0.144589	27 C -0.199336	27 C -0.194348	27 C -0.174458
28 H 0.113348	28 H 0.121308	28 H 0.135857	28 H 0.126597	28 H 0.141670	28 H 0.151027
29 H 0.063577	29 H 0.055655	29 H 0.029964	29 H 0.087611	29 H 0.079318	29 H 0.052987
30 C -0.178408	30 C -0.177621	30 C -0.172182	30 C -0.210889	30 C -0.211214	30 C -0.203924
31 H 0.134765	31 H 0.141050	31 H 0.142425	31 H 0.146986	31 H 0.165075	31 H 0.156668
32 H 0.111421	32 H 0.120817	32 H 0.142361	32 H 0.136065	32 H 0.151845	32 H 0.167920
33 C -0.052864	33 C -0.052796	33 C -0.050440	33 C -0.092329	33 C -0.093873	33 C -0.090671
34 H 0.050926	34 H 0.039339	34 H 0.012535	34 H 0.072104	34 H 0.053304	34 H 0.031654
35 H 0.043112	35 H 0.027750	35 H -0.016504	35 H 0.059533	35 H 0.039170	35 H -0.001949
36 H 0.094642	36 H 0.098506	36 H 0.108106	36 H 0.120071	36 H 0.126095	36 H 0.133366
37 H 0.050428	37 H 0.040150	37 H 0.013702	37 H 0.066695	37 H 0.051396	37 H 0.028479
38 H 0.101157	38 H 0.107732	38 H 0.116019	38 H 0.121576	38 H 0.136387	38 H 0.137516
39 C -0.162302	39 C -0.157619	39 C -0.134337	39 C -0.195125	39 C -0.194413	39 C -0.166280
40 H 0.090049	40 H 0.091375	40 H 0.089057	40 H 0.110637	40 H 0.115564	40 H 0.110058
41 H 0.053742	41 H 0.042576	41 H 0.013767	41 H 0.068048	41 H 0.051316	41 H 0.027636
42 C -0.173662	42 C -0.170949	42 C -0.156931	42 C -0.212800	42 C -0.211046	42 C -0.192103
43 H 0.069981	43 H 0.055563	43 H -0.002520	43 H 0.086425	43 H 0.076905	43 H 0.012452
44 H 0.113916	44 H 0.114100	44 H 0.087403	44 H 0.138046	44 H 0.153821	44 H 0.112080
45 C -0.163880	45 C -0.147319	45 C -0.057076	45 C -0.204211	45 C -0.203107	45 C -0.115961
46 H 0.056273	46 H 0.026515	46 H -0.107905	46 H 0.077601	46 H 0.063765	46 H -0.066519
47 H 0.099296	47 H 0.090479	47 H 0.036583	47 H 0.118986	47 H 0.126834	47 H 0.064092
48 C -0.155334	48 C -0.123401	48 C 0.003197	48 C -0.203367	48 C -0.197415	48 C -0.035843
49 H 0.109608	49 H 0.081703	49 H -0.063584	49 H 0.129367	49 H 0.137850	49 H -0.043806
50 H 0.064199	50 H 0.004689	50 H -0.315026	50 H 0.084316	50 H 0.072393	50 H -0.287925
51 C -0.306766	51 C -0.179369	51 C 0.419161	51 C -0.351810	51 C -0.348294	51 C 0.395193
52 H 0.066603	52 H -0.063881	52 H -0.661739	52 H 0.083020	52 H 0.066222	52 H -0.665144
53 H 0.107887	53 H 0.030446	53 H -0.345711	53 H 0.125812	53 H 0.130441	53 H -0.356784
54 F -0.288213	54 F -0.239396	54 F 0.001689	54 F -0.312621	54 F -0.296806	54 F -0.028636
55 H 0.107160	55 H 0.116697	55 H 0.147401	55 H 0.126182	55 H 0.137145	55 H 0.167323
56 H 0.061751	56 H 0.057666	56 H 0.059859	56 H 0.084673	56 H 0.072404	56 H 0.080923
57 H 0.134522	57 H 0.154146	57 H 0.228146	57 H 0.162326	57 H 0.176846	57 H 0.255667
58 H 0.070274	58 H 0.066245	58 H 0.070684	58 H 0.088398	58 H 0.074917	58 H 0.086459
59 H 0.041956	59 H -0.123118	59 H -0.882386	59 H 0.062133	59 H 0.032839	59 H -0.867516

Table S3. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure 1) of Molecule 3 (Dihedral Angle around 70°)

MOLECULE 3					
B3LYP			M062X		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
1 C -0.067443	1 C -0.046667	1 C 0.060786	1 C -0.093822	1 C -0.083519	1 C 0.055224
2 C -0.113521	2 C -0.107404	2 C -0.075726	2 C -0.136147	2 C -0.135364	2 C -0.106758
3 C 0.057973	3 C 0.071272	3 C 0.134164	3 C 0.031484	3 C 0.033625	3 C 0.114160
4 C -0.111785	4 C -0.105381	4 C -0.078000	4 C -0.134557	4 C -0.132539	4 C -0.107411
5 C -0.069301	5 C -0.052562	5 C 0.020684	5 C -0.096164	5 C -0.089185	5 C 0.001412
6 H 0.166290	6 H 0.214791	6 H 0.368389	6 H 0.203091	6 H 0.236317	6 H 0.402013
7 H 0.108997	7 H 0.139560	7 H 0.250437	7 H 0.142039	7 H 0.156139	7 H 0.284662
8 H 0.050030	8 H 0.056544	8 H 0.106688	8 H 0.082293	8 H 0.067615	8 H 0.141712
9 H 0.115159	9 H 0.143576	9 H 0.250154	9 H 0.151915	9 H 0.162923	9 H 0.287308
10 C 0.062967	10 C 0.061770	10 C 0.055163	10 C 0.035153	10 C 0.035135	10 C 0.018950
11 C -0.109093	11 C -0.102437	11 C -0.074887	11 C -0.127191	11 C -0.122960	11 C -0.093666
12 C -0.109632	12 C -0.103168	12 C -0.073534	12 C -0.127596	12 C -0.124423	12 C -0.091954
13 C -0.136156	13 C -0.136120	13 C -0.131337	13 C -0.159015	13 C -0.162189	13 C -0.156793
14 H 0.109646	14 H 0.126734	14 H 0.185311	14 H 0.144685	14 H 0.157852	14 H 0.217319
15 C -0.143737	15 C -0.142480	15 C -0.134097	15 C -0.168153	15 C -0.169739	15 C -0.161201
16 H 0.106440	16 H 0.123791	16 H 0.185395	16 H 0.141767	16 H 0.154032	16 H 0.217808
17 C 0.125588	17 C 0.126556	17 C 0.137676	17 C 0.080596	17 C 0.077207	17 C 0.090788
18 H 0.053855	18 H 0.054871	18 H 0.072688	18 H 0.087388	18 H 0.077355	18 H 0.102935
19 H 0.056854	19 H 0.061581	19 H 0.092375	19 H 0.091717	19 H 0.084453	19 H 0.124338
20 C -0.243421	20 C -0.244421	20 C -0.248632	20 C -0.269026	20 C -0.268956	20 C -0.274495

Table S3. *Continue*

MOLECULE 3					
B3LYP			M062X		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
21 C -0.161682	21 C -0.160666	21 C -0.159880	21 C -0.194284	21 C -0.190892	21 C -0.190821
22 C -0.039808	22 C -0.037983	22 C -0.031916	22 C -0.078272	22 C -0.076376	22 C -0.070668
23 C -0.176948	23 C -0.177419	23 C -0.178071	23 C -0.206217	23 C -0.207448	23 C -0.208568
24 C -0.168650	24 C -0.164682	24 C -0.151219	24 C -0.201532	24 C -0.196843	24 C -0.181882
25 H 0.065646	25 H 0.065029	25 H 0.064273	25 H 0.084334	25 H 0.082665	25 H 0.083012
26 C -0.185328	26 C -0.186920	26 C -0.189181	26 C -0.218983	26 C -0.222650	26 C -0.224137
27 H 0.091374	27 H 0.093065	27 H 0.095077	27 H 0.108908	27 H 0.113507	27 H 0.112565
28 H 0.152245	28 H 0.163319	28 H 0.185471	28 H 0.171651	28 H 0.193866	28 H 0.209359
29 C -0.163555	29 C -0.156750	29 C -0.129726	29 C -0.196596	29 C -0.189624	29 C -0.161532
30 H 0.077837	30 H 0.073491	30 H 0.056992	30 H 0.095500	30 H 0.092420	30 H 0.074055
31 H 0.053702	31 H 0.038413	31 H -0.016134	31 H 0.077177	31 H 0.062422	31 H 0.005949
32 C -0.048680	32 C -0.047384	32 C -0.040249	32 C -0.087592	32 C -0.087012	32 C -0.077878
33 H 0.104554	33 H 0.111738	33 H 0.131089	33 H 0.130237	33 H 0.139965	33 H 0.157630
34 H 0.081739	34 H 0.083216	34 H 0.087576	34 H 0.099272	34 H 0.100439	34 H 0.105847
35 H 0.027177	35 H 0.004575	35 H -0.063867	35 H 0.047502	35 H 0.017817	35 H -0.046666
36 H 0.066015	36 H 0.060504	36 H 0.042420	36 H 0.083545	36 H 0.076545	36 H 0.060612
37 H 0.072703	37 H 0.068292	37 H 0.049008	37 H 0.091941	37 H 0.091095	37 H 0.067125
38 C -0.165499	38 C -0.160611	38 C -0.138767	38 C -0.199473	38 C -0.199021	38 C -0.171146
39 H 0.100720	39 H 0.105368	39 H 0.112043	39 H 0.121852	39 H 0.130589	39 H 0.134663
40 H 0.078133	40 H 0.076485	40 H 0.069269	40 H 0.093624	40 H 0.090753	40 H 0.087129
41 C -0.168306	41 C -0.161304	41 C -0.115917	41 C -0.206726	41 C -0.201026	41 C -0.164305
42 H 0.059621	42 H 0.035321	42 H -0.084171	42 H 0.075778	42 H 0.057755	42 H -0.051823
43 H 0.084445	43 H 0.066815	43 H -0.025445	43 H 0.107627	43 H 0.103034	43 H 0.005282
44 C -0.159422	44 C -0.123367	44 C 0.044279	44 C -0.199380	44 C -0.184623	44 C 0.001259
45 H 0.105613	45 H 0.089138	45 H 0.017068	45 H 0.125600	45 H 0.128283	45 H 0.041685
46 H 0.029060	46 H -0.045638	46 H -0.378604	46 H 0.049602	46 H 0.006137	46 H -0.361242
47 C -0.158170	47 C -0.116424	47 C 0.023211	47 C -0.206496	47 C -0.188768	47 C 0.000923
48 H 0.133909	48 H 0.114756	48 H 0.044397	48 H 0.154423	48 H 0.162758	48 H 0.058784
49 H 0.057441	49 H -0.025470	49 H -0.380851	49 H 0.077278	49 H 0.040941	49 H -0.376567
50 C -0.307936	50 C -0.191737	50 C 0.252090	50 C -0.353174	50 C -0.313761	50 C 0.213565
51 H 0.072282	51 H -0.042244	51 H -0.522706	51 H 0.093245	51 H 0.049896	51 H -0.525982
52 H 0.120128	52 H 0.056493	52 H -0.180830	52 H 0.138371	52 H 0.126547	52 H -0.168067
53 H 0.043440	53 H -0.129734	53 H -0.766152	53 H 0.059060	53 H -0.019005	53 H -0.755112
54 C -0.101853	54 C -0.113493	54 C -0.142563	54 C -0.140548	54 C -0.146479	54 C -0.191693
55 H 0.078836	55 H 0.079245	55 H 0.087809	55 H 0.100176	55 H 0.095253	55 H 0.107895
56 H 0.120090	56 H 0.131177	56 H 0.171723	56 H 0.147428	56 H 0.155359	56 H 0.198510
57 H 0.050227	57 H 0.039341	57 H 0.010192	57 H 0.072192	57 H 0.055649	57 H 0.029289
58 H 0.091992	58 H 0.093395	58 H 0.097373	58 H 0.108024	58 H 0.110161	58 H 0.113266
59 Cl 0.077198	59 Cl 0.252243	59 Cl 0.951192	59 Cl 0.094469	59 Cl 0.185891	59 Cl 0.993334

Table S4. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure 1) of Molecule 4 (Dihedral Angle around 70°)

MOLECULE 4					
B3LYP			M062X		
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
1 C -0.079222	1 C -0.065938	1 C 0.000227	1 C -0.097361	1 C -0.095085	1 C -0.012478
2 C -0.119750	2 C -0.113971	2 C -0.083215	2 C -0.142955	2 C -0.141433	2 C -0.111737
3 C 0.071510	3 C 0.081060	3 C 0.141055	3 C 0.044477	3 C 0.041780	3 C 0.122517
4 C -0.122977	4 C -0.117901	4 C -0.081516	4 C -0.146480	4 C -0.147639	4 C -0.113381
5 C -0.075396	5 C -0.056098	5 C 0.056798	5 C -0.091217	5 C -0.083996	5 C 0.064260
6 C 0.107483	6 C 0.121749	6 C 0.194593	6 C 0.058817	6 C 0.066890	6 C 0.148462
7 H 0.104881	7 H 0.122076	7 H 0.216494	7 H 0.143174	7 H 0.138999	7 H 0.256444
8 H 0.044635	8 H 0.041435	8 H 0.087457	8 H 0.076945	8 H 0.046758	8 H 0.124114
9 H 0.123810	9 H 0.153238	9 H 0.273098	9 H 0.157274	9 H 0.168658	9 H 0.307702
10 H 0.178229	10 H 0.224426	10 H 0.381174	10 H 0.216085	10 H 0.245576	10 H 0.415311
11 C 0.059930	11 C 0.059292	11 C 0.054105	11 C 0.031339	11 C 0.032807	11 C 0.015380
12 C -0.108434	12 C -0.102498	12 C -0.068514	12 C -0.126568	12 C -0.123880	12 C -0.085329
13 C -0.106683	13 C -0.100995	13 C -0.072239	13 C -0.124825	13 C -0.122665	13 C -0.091702
14 C -0.136776	14 C -0.137470	14 C -0.129252	14 C -0.159868	14 C -0.164727	14 C -0.155412
15 H 0.121847	15 H 0.142722	15 H 0.218697	15 H 0.156933	15 H 0.173302	15 H 0.250793
16 C -0.145901	16 C -0.145336	16 C -0.136760	16 C -0.167822	16 C -0.170186	16 C -0.161614
17 H 0.095872	17 H 0.105881	17 H 0.152160	17 H 0.130554	17 H 0.134232	17 H 0.183415
18 C 0.131514	18 C 0.132158	18 C 0.145793	18 C 0.087828	18 C 0.083801	18 C 0.099953
19 H 0.079465	19 H 0.088058	19 H 0.139868	19 H 0.112970	19 H 0.110251	19 H 0.171041
20 H 0.039885	20 H 0.032443	20 H 0.042391	20 H 0.072406	20 H 0.048924	20 H 0.071079

Table S4. *Continue*

MOLECULE 4											
B3LYP				M062X							
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.038a.u.
21 C -0.244342	21 C -0.245392	21 C -0.250832	21 C -0.271415	21 C -0.270975	21 C -0.277614	22 C -0.171221	22 C -0.170264	22 C -0.172239	22 C -0.202877	22 C -0.199485	22 C -0.203578
23 C -0.036082	23 C -0.032759	23 C -0.022683	23 C -0.074816	23 C -0.070073	23 C -0.059308	24 C -0.170634	24 C -0.167762	24 C -0.157926	24 C -0.202004	24 C -0.198924	24 C -0.189082
25 C -0.178817	25 C -0.180040	25 C -0.183382	25 C -0.208850	25 C -0.211222	25 C -0.215018	26 H 0.037781	26 H 0.023485	26 H -0.013776	26 H 0.057013	26 H 0.036989	26 H 0.002488
27 C -0.166809	27 C -0.161401	27 C -0.140111	27 C -0.198619	27 C -0.192924	27 C -0.169328	28 H 0.114464	28 H 0.124080	28 H 0.142873	28 H 0.127471	28 H 0.143522	28 H 0.158122
29 H 0.058207	29 H 0.046353	29 H 0.005501	29 H 0.082033	29 H 0.070223	29 H 0.027754	30 C -0.178659	30 C -0.178038	30 C -0.172170	30 C -0.211290	30 C -0.211735	30 C -0.204076
31 H 0.135877	31 H 0.145426	31 H 0.156088	31 H 0.148006	31 H 0.168021	31 H 0.171409	32 H 0.111191	32 H 0.120707	32 H 0.141029	32 H 0.135962	32 H 0.151169	32 H 0.166925
33 C -0.052757	33 C -0.052953	33 C -0.050832	33 C -0.092564	33 C -0.094402	33 C -0.091574	34 H 0.051658	34 H 0.038792	34 H 0.008175	34 H 0.072788	34 H 0.053808	34 H 0.027135
35 H 0.040597	35 H 0.022758	35 H -0.029761	35 H 0.056946	35 H 0.034651	35 H -0.015397	36 H 0.100036	36 H 0.106211	36 H 0.121130	36 H 0.125591	36 H 0.134254	36 H 0.146915
37 H 0.049523	37 H 0.037274	37 H 0.003948	37 H 0.065687	37 H 0.049142	37 H 0.018358	38 H 0.102940	38 H 0.111442	38 H 0.123224	38 H 0.123538	38 H 0.139949	38 H 0.145220
39 C -0.162947	39 C -0.158470	39 C -0.133506	39 C -0.195800	39 C -0.195217	39 C -0.165599	40 H 0.095102	40 H 0.098749	40 H 0.101279	40 H 0.115710	40 H 0.123182	40 H 0.122519
41 H 0.052445	41 H 0.039743	41 H 0.006452	41 H 0.066712	41 H 0.048865	41 H 0.020595	42 C -0.173983	42 C -0.171130	42 C -0.154380	42 C -0.213032	42 C -0.211232	42 C -0.190302
43 H 0.065289	43 H 0.048643	43 H -0.020725	43 H 0.081673	43 H 0.069506	43 H -0.004233	44 H 0.115591	44 H 0.117587	44 H 0.090900	44 H 0.139688	44 H 0.156531	44 H 0.115728
45 C -0.164469	45 C -0.149391	45 C -0.060348	45 C -0.204811	45 C -0.204032	45 C -0.117726	46 H 0.058363	46 H 0.029764	46 H -0.108946	46 H 0.079692	46 H 0.066727	46 H -0.068262
47 H 0.105175	47 H 0.100097	47 H 0.052779	47 H 0.124952	47 H 0.135727	47 H 0.078950	48 C -0.155788	48 C -0.122144	48 C 0.035207	48 C -0.203556	48 C -0.197505	48 C 0.001474
49 H 0.108850	49 H 0.081732	49 H -0.075686	49 H 0.128440	49 H 0.136552	49 H -0.056512	50 H 0.058207	50 H -0.006057	50 H -0.381451	50 H 0.078159	50 H 0.062847	50 H -0.364282
51 C -0.306715	51 C -0.191836	51 C 0.383664	51 C -0.351801	51 C -0.348156	51 C 0.352818	52 H 0.068169	52 H -0.050707	52 H -0.633088	52 H 0.084568	52 H 0.068429	52 H -0.638184
53 H 0.114632	53 H 0.051021	53 H -0.285076	53 H 0.132735	53 H 0.140652	53 H -0.283848	54 C 0.093150	54 C 0.148654	54 C 0.447403	54 C 0.106146	54 C 0.109642	54 C 0.446040
55 N -0.242951	55 N -0.172790	55 N 0.150718	55 N -0.246351	55 N -0.209910	55 N 0.169952	56 H 0.129507	56 H 0.143833	56 H 0.198721	56 H 0.157050	56 H 0.168078	56 H 0.225975
57 H 0.070920	57 H 0.064113	57 H 0.057797	57 H 0.089108	57 H 0.074714	57 H 0.073312	58 H 0.106568	58 H 0.115122	58 H 0.140982	58 H 0.125617	58 H 0.135859	58 H 0.160981
59 H 0.057043	59 H 0.047128	59 H 0.028021	59 H 0.079747	59 H 0.063469	59 H 0.048191	60 H 0.040965	60 H -0.115910	60 H -0.881388	60 H 0.061051	60 H 0.030919	60 H -0.865760

Table S5. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S5) of Molecule 1 (Dihedral Angle around 1800°)

MOLECULE 1											
B3LYP				M062X							
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.
1 C -0.089850	1 C -0.075687	1 C -0.004401	1 C -0.125295	1 C -0.118028	1 C -0.041528	2 C -0.114507	2 C -0.100713	2 C -0.061717	2 C -0.135688	2 C -0.129103	2 C -0.086613
3 C 0.058189	3 C 0.077449	3 C 0.157857	3 C 0.031313	3 C 0.039882	3 C 0.142973	4 C -0.114708	4 C -0.102058	4 C -0.065015	4 C -0.135981	4 C -0.129963	4 C -0.088442
5 C -0.088202	5 C -0.074716	5 C -0.017851	5 C -0.123900	5 C -0.117318	5 C -0.060166	6 H 0.135059	6 H 0.193716	6 H 0.353211	6 H 0.170796	6 H 0.212363	6 H 0.387373
7 H 0.090874	7 H 0.128195	7 H 0.236136	7 H 0.123084	7 H 0.143876	7 H 0.272877	8 H 0.054285	8 H 0.076828	8 H 0.152947	8 H 0.086122	8 H 0.090128	8 H 0.191578
9 H 0.106558	9 H 0.154853	9 H 0.292889	9 H 0.142198	9 H 0.172266	9 H 0.329571	10 C 0.063307	10 C 0.061587	10 C 0.058045	10 C 0.034868	10 C 0.033669	10 C 0.012277
11 C -0.109205	11 C -0.097571	11 C -0.051592	11 C -0.128275	11 C -0.120724	11 C -0.067848	12 C -0.109926	12 C -0.099894	12 C -0.063775	12 C -0.129319	12 C -0.123279	12 C -0.082302
13 C -0.133439	13 C -0.131759	13 C -0.122225	13 C -0.156494	13 C -0.158077	13 C -0.150136	14 H 0.122568	14 H 0.153758	14 H 0.244670	14 H 0.157582	14 H 0.182073	14 H 0.275427
15 C -0.129502	15 C -0.126191	15 C -0.114214	15 C -0.151988	15 C -0.151230	15 C -0.141639	16 H 0.088406	16 H 0.104849	16 H 0.159648	16 H 0.123318	16 H 0.132318	16 H 0.190844

Table S5. *Continue*

MOLECULE 1											
B3LYP						M062X					
FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.	FIELD = 0.012a.u.	FIELD = 0.018a.u.	FIELD = 0.036a.u.
17 C 0.119061	17 C 0.127339	17 C 0.157248	17 C 0.078437	17 C 0.082400	17 C 0.114258	17 C 0.119061	17 C 0.127339	17 C 0.157248	17 C 0.078437	17 C 0.082400	17 C 0.114258
18 H 0.065861	18 H 0.085952	18 H 0.152530	18 H 0.100668	18 H 0.107654	18 H 0.184288	18 H 0.065861	18 H 0.085952	18 H 0.152530	18 H 0.100668	18 H 0.107654	18 H 0.184288
19 H 0.036815	19 H 0.043629	19 H 0.075203	19 H 0.071169	19 H 0.063589	19 H 0.105587	19 H 0.036815	19 H 0.043629	19 H 0.075203	19 H 0.071169	19 H 0.063589	19 H 0.105587
20 C -0.252359	20 C -0.257806	20 C -0.272715	20 C -0.278287	20 C -0.283601	20 C -0.300083	20 C -0.252359	20 C -0.257806	20 C -0.272715	20 C -0.278287	20 C -0.283601	20 C -0.300083
21 C -0.158604	21 C -0.161337	21 C -0.170817	21 C -0.188437	21 C -0.189750	21 C -0.199540	21 C -0.158604	21 C -0.161337	21 C -0.170817	21 C -0.188437	21 C -0.189750	21 C -0.199540
22 C -0.049232	22 C -0.050399	22 C -0.053065	22 C -0.090287	22 C -0.092147	22 C -0.095716	22 C -0.049232	22 C -0.050399	22 C -0.053065	22 C -0.090287	22 C -0.092147	22 C -0.095716
23 C -0.173856	23 C -0.174017	23 C -0.173989	23 C -0.209970	23 C -0.209623	23 C -0.209391	23 C -0.173856	23 C -0.174017	23 C -0.173989	23 C -0.209970	23 C -0.209623	23 C -0.209391
24 C -0.173452	24 C -0.171823	24 C -0.166942	24 C -0.206531	24 C -0.204618	24 C -0.198378	24 C -0.173452	24 C -0.171823	24 C -0.166942	24 C -0.206531	24 C -0.204618	24 C -0.198378
25 H 0.088674	25 H 0.098983	25 H 0.129932	25 H 0.108786	25 H 0.118377	25 H 0.151429	25 H 0.088674	25 H 0.098983	25 H 0.129932	25 H 0.108786	25 H 0.118377	25 H 0.151429
26 C -0.179590	26 C -0.179571	26 C -0.178434	26 C -0.213193	26 C -0.214215	26 C -0.213083	26 C -0.179590	26 C -0.179571	26 C -0.178434	26 C -0.213193	26 C -0.214215	26 C -0.213083
27 H 0.072176	27 H 0.064617	27 H 0.041275	27 H 0.089910	27 H 0.083525	27 H 0.057431	27 H 0.072176	27 H 0.064617	27 H 0.041275	27 H 0.089910	27 H 0.083525	27 H 0.057431
28 H 0.131014	28 H 0.143919	28 H 0.178256	28 H 0.155463	28 H 0.173519	28 H 0.205052	28 H 0.131014	28 H 0.143919	28 H 0.178256	28 H 0.155463	28 H 0.173519	28 H 0.205052
29 C -0.171150	29 C -0.167666	29 C -0.155515	29 C -0.205444	29 C -0.202562	29 C -0.189475	29 C -0.171150	29 C -0.167666	29 C -0.155515	29 C -0.205444	29 C -0.202562	29 C -0.189475
30 H 0.066948	30 H 0.056071	30 H 0.022492	30 H 0.084230	30 H 0.074241	30 H 0.037803	30 H 0.066948	30 H 0.056071	30 H 0.022492	30 H 0.084230	30 H 0.074241	30 H 0.037803
31 H 0.095412	31 H 0.095825	31 H 0.094646	31 H 0.120751	31 H 0.124261	31 H 0.120291	31 H 0.095412	31 H 0.095825	31 H 0.094646	31 H 0.120751	31 H 0.124261	31 H 0.120291
32 C -0.044847	32 C -0.041363	32 C -0.028087	32 C -0.082849	32 C -0.079474	32 C -0.064064	32 C -0.044847	32 C -0.041363	32 C -0.028087	32 C -0.082849	32 C -0.079474	32 C -0.064064
33 H 0.067698	33 H 0.062652	33 H 0.048205	33 H 0.091776	33 H 0.085310	33 H 0.071614	33 H 0.067698	33 H 0.062652	33 H 0.048205	33 H 0.091776	33 H 0.085310	33 H 0.071614
34 H 0.096880	34 H 0.104718	34 H 0.126782	34 H 0.115049	34 H 0.122950	34 H 0.146751	34 H 0.096880	34 H 0.104718	34 H 0.126782	34 H 0.115049	34 H 0.122950	34 H 0.146751
35 H 0.038878	35 H 0.022830	35 H -0.022085	35 H 0.059504	35 H 0.037985	35 H -0.004685	35 H 0.038878	35 H 0.022830	35 H -0.022085	35 H 0.059504	35 H 0.037985	35 H -0.004685
36 H 0.089095	36 H 0.094367	36 H 0.108687	36 H 0.107422	36 H 0.112357	36 H 0.128724	36 H 0.089095	36 H 0.094367	36 H 0.108687	36 H 0.107422	36 H 0.112357	36 H 0.128724
37 H 0.053283	37 H 0.038399	37 H -0.007629	37 H 0.071675	37 H 0.059073	37 H 0.007982	37 H 0.053283	37 H 0.038399	37 H -0.007629	37 H 0.071675	37 H 0.059073	37 H 0.007982
38 C -0.162293	38 C -0.154428	38 C -0.128231	38 C -0.195799	38 C -0.191665	38 C -0.160584	38 C -0.162293	38 C -0.154428	38 C -0.128231	38 C -0.195799	38 C -0.191665	38 C -0.160584
39 H 0.068342	39 H 0.059982	39 H 0.033209	39 H 0.087990	39 H 0.080675	39 H 0.053517	39 H 0.068342	39 H 0.059982	39 H 0.033209	39 H 0.087990	39 H 0.080675	39 H 0.053517
40 H 0.094944	40 H 0.099736	40 H 0.108448	40 H 0.111250	40 H 0.116478	40 H 0.128546	40 H 0.094944	40 H 0.099736	40 H 0.108448	40 H 0.111250	40 H 0.116478	40 H 0.128546
41 C -0.166893	41 C -0.159436	41 C -0.124633	41 C -0.205768	41 C -0.199094	41 C -0.168123	41 C -0.166893	41 C -0.159436	41 C -0.124633	41 C -0.205768	41 C -0.199094	41 C -0.168123
42 H 0.089727	42 H 0.076488	42 H 0.023763	42 H 0.107270	42 H 0.101080	42 H 0.045437	42 H 0.089727	42 H 0.076488	42 H 0.023763	42 H 0.107270	42 H 0.101080	42 H 0.045437
43 H 0.066337	43 H 0.034621	43 H -0.094778	43 H 0.088897	43 H 0.069182	43 H -0.058667	43 H 0.066337	43 H 0.034621	43 H -0.094778	43 H 0.088897	43 H 0.069182	43 H -0.058667
44 C -0.156472	44 C -0.099395	44 C 0.127457	44 C -0.195042	44 C -0.163202	44 C 0.070789	44 C -0.156472	44 C -0.099395	44 C 0.127457	44 C -0.195042	44 C -0.163202	44 C 0.070789
45 H 0.071182	45 H 0.020393	45 H -0.162249	45 H 0.089795	45 H 0.061342	45 H -0.124235	45 H 0.071182	45 H 0.020393	45 H -0.162249	45 H 0.089795	45 H 0.061342	45 H -0.124235
46 H 0.025161	46 H -0.073613	46 H -0.450424	46 H 0.045466	46 H -0.019002	46 H -0.431529	46 H 0.025161	46 H -0.073613	46 H -0.450424	46 H 0.045466	46 H -0.019002	46 H -0.431529
47 C -0.160140	47 C -0.127260	47 C -0.073968	47 C -0.209332	47 C -0.187952	47 C -0.098617	47 C -0.160140	47 C -0.127260	47 C -0.073968	47 C -0.209332	47 C -0.187952	47 C -0.098617
48 H 0.135162	48 H 0.113489	48 H 0.065019	48 H 0.155574	48 H 0.154980	48 H 0.079119	48 H 0.135162	48 H 0.113489	48 H 0.065019	48 H 0.155574	48 H 0.154980	48 H 0.079119
49 H 0.092559	49 H 0.040167	49 H -0.105670	49 H 0.113604	49 H 0.088445	49 H -0.086419	49 H 0.092559	49 H 0.040167	49 H -0.105670	49 H 0.113604	49 H 0.088445	49 H -0.086419
50 C -0.308817	50 C -0.162232	50 C 0.291342	50 C -0.353607	50 C -0.277849	50 C 0.272477	50 C -0.308817	50 C -0.162232	50 C 0.291342	50 C -0.353607	50 C -0.277849	50 C 0.272477
51 H 0.093091	51 H -0.015951	51 H -0.378420	51 H 0.114625	51 H 0.060996	51 H -0.381692	51 H 0.093091	51 H -0.015951	51 H -0.378420	51 H 0.114625	51 H 0.060996	51 H -0.381692
52 H 0.085639	52 H -0.038066	52 H -0.426305	52 H 0.102746	52 H 0.036363	52 H -0.445870	52 H 0.085639	52 H -0.038066	52 H -0.426305	52 H 0.102746	52 H 0.036363	52 H -0.445870
53 H 0.043424	53 H -0.161559	53 H -0.763802	53 H 0.059015	53 H -0.064049	53 H -0.752872	53 H 0.043424	53 H -0.161559	53 H -0.763802	53 H 0.059015	53 H -0.064049	53 H -0.752872
54 C -0.074820	54 C -0.037784	54 C 0.136528	54 C -0.110206	54 C -0.086493	54 C 0.143556	54 C -0.074820	54 C -0.037784	54 C 0.136528	54 C -0.110206	54 C -0.086493	54 C 0.143556
55 H 0.145496	55 H 0.214283	55 H 0.392651	55 H 0.181338	55 H 0.230608	55 H 0.429078	55 H 0.145496	55 H 0.214283	55 H 0.392651	55 H 0.181338	55 H 0.230608	55 H 0.429078
56 H 0.093161	56 H 0.101952	56 H 0.132738	56 H 0.112663	56 H 0.115486	56 H 0.150935	56 H 0.093161	56 H 0.101952	56 H 0.132738	56 H 0.112663	56 H 0.115486	56 H 0.150935
57 H 0.106239	57 H 0.123444	57 H 0.177633	57 H 0.129560	57 H 0.141371	57 H 0.200628	57 H 0.106239	57 H 0.123444	57 H 0.177633	57 H 0.129560	57 H 0.141371	57 H 0.200628
58 H 0.095512	58 H 0.098177	58 H 0.106504	58 H 0.115537	58 H 0.118716	58 H 0.125826	58 H 0.095512	58 H 0.098177	58 H 0.106504	58 H 0.115537	58 H 0.118716	58 H 0.125826
59 H 0.074848	59 H 0.069031	59 H 0.052600	59 H 0.092240	59 H 0.085479	59 H 0.067665	59 H 0.074848	59 H 0.069031	59 H 0.052600	59 H 0.092240	59 H 0.085479	59 H 0.067665

Table S6. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S5) of Molecule 2 (Dihedral Angle around 180°)

MOLECULE 2											
B3LYP						M062X					
FIELD = 0.018a.u.	FIELD = 0.024a.u.	FIELD = 0.048a.u.	FIELD = 0.018a.u.	FIELD = 0.024a.u.	FIELD = 0.05a.u.	FIELD = 0.018a.u.	FIELD = 0.024a.u.	FIELD = 0.048a.u.	FIELD = 0.018a.u.	FIELD = 0.024a.u.	FIELD = 0.05a.u.
1 C -0.148111	1 C -0.127105	1 C -0.036375	1 C -0.179688	1 C -0.170026	1 C -0.058072	1 C -0.148111	1 C -0.127105	1 C -0.036375	1 C -0.179688	1 C -0.170026	1 C -0.058072
2 C -0.109499	2 C -0.100488	2 C -0.068956	2 C -0.129804	2 C -0.126063	2 C -0.096114	2 C -0.109499	2 C -0.100488	2 C -0.068956	2 C -0.129804	2 C -0.126063	2 C -0.096114
3 C 0.052565	3 C 0.070912	3 C 0.154454	3 C 0.024703	3 C 0.030914	3 C 0.141990	3 C 0.052565	3 C 0.070912	3 C 0.154454	3 C 0.024703	3 C 0.030914	3 C 0.141990
4 C -0.113887	4 C -0.106427	4 C -0.080230	4 C -0.134449	4 C -0.132434	4 C -0.110634	4 C -0.113887	4 C -0.106427	4 C -0.080230	4 C -0.134449	4 C -0.132434	4 C -0.110634
5 C -0.141446	5 C -0.116750	5 C -0.004161	5 C -0.172577	5 C -0.159502	5 C -0.016497	5 C -0.141446	5 C -0.116750	5 C -0.004161	5 C -0.172577	5 C -0.159502	5 C -0.016497

Table S6. *Continue*

MOLECULE 2													
B3LYP							M062X						
FIELD = 0.018a.u.		FIELD = 0.024a.u.		FIELD = 0.048a.u.		FIELD = 0.018a.u.		FIELD = 0.024a.u.		FIELD = 0.05a.u.			
6 C	0.416785	6 C	0.449744	6 C	0.589288	6 C	0.424206	6 C	0.445708	6 C	0.621645		
7 H	0.137657	7 H	0.181358	7 H	0.327338	7 H	0.175616	7 H	0.200425	7 H	0.368614		
8 H	0.075069	8 H	0.100897	8 H	0.191937	8 H	0.107326	8 H	0.114475	8 H	0.228911		
9 H	0.083025	9 H	0.111303	9 H	0.209154	9 H	0.115889	9 H	0.125816	9 H	0.246893		
10 H	0.158680	10 H	0.207803	10 H	0.369315	10 H	0.196535	10 H	0.227137	10 H	0.410247		
11 C	0.065044	11 C	0.062791	11 C	0.055635	11 C	0.037041	11 C	0.035916	11 C	0.012891		
12 C	-0.108113	12 C	-0.097485	12 C	-0.039500	12 C	-0.126380	12 C	-0.119120	12 C	-0.050111		
13 C	-0.108133	13 C	-0.100809	13 C	-0.072056	13 C	-0.127338	13 C	-0.122788	13 C	-0.092058		
14 C	-0.136625	14 C	-0.135076	14 C	-0.120624	14 C	-0.159546	14 C	-0.161389	14 C	-0.146016		
15 H	0.163108	15 H	0.196418	15 H	0.314135	15 H	0.198693	15 H	0.226472	15 H	0.350197		
16 C	-0.124238	16 C	-0.119962	16 C	-0.100886	16 C	-0.146641	16 C	-0.143505	16 C	-0.124541		
17 H	0.052640	17 H	0.053059	17 H	0.056147	17 H	0.087535	17 H	0.081078	17 H	0.082663		
18 C	0.118203	18 C	0.124851	18 C	0.149545	18 C	0.079215	18 C	0.082205	18 C	0.107455		
19 H	0.097917	19 H	0.124904	19 H	0.222729	19 H	0.133241	19 H	0.148016	19 H	0.256842		
20 H	-0.011703	20 H	-0.019743	20 H	-0.052030	20 H	0.021966	20 H	-0.001054	20 H	-0.035591		
21 C	-0.253550	21 C	-0.257344	21 C	-0.268732	21 C	-0.281414	21 C	-0.285576	21 C	-0.298258		
22 C	-0.157138	22 C	-0.156964	22 C	-0.154372	22 C	-0.186374	22 C	-0.184898	22 C	-0.181345		
23 C	-0.039944	23 C	-0.036118	23 C	-0.018674	23 C	-0.078457	23 C	-0.074326	23 C	-0.053713		
24 C	-0.183950	24 C	-0.187407	24 C	-0.198831	24 C	-0.221794	24 C	-0.224970	24 C	-0.239087		
25 C	-0.161550	25 C	-0.157234	25 C	-0.136464	25 C	-0.198027	25 C	-0.193376	25 C	-0.169700		
26 H	0.017429	26 H	0.003117	26 H	-0.055972	26 H	0.037346	26 H	0.018884	26 H	-0.046738		
27 C	-0.179925	27 C	-0.179409	27 C	-0.173420	27 C	-0.213510	27 C	-0.213993	27 C	-0.207747		
28 H	0.141174	28 H	0.154690	28 H	0.206420	28 H	0.159229	28 H	0.175951	28 H	0.233458		
29 H	0.129314	29 H	0.139780	29 H	0.179679	29 H	0.155855	29 H	0.169698	29 H	0.213755		
30 C	-0.158686	30 C	-0.151464	30 C	-0.111405	30 C	-0.188777	30 C	-0.180777	30 C	-0.142447		
31 H	0.126216	31 H	0.135049	31 H	0.169160	31 H	0.144017	31 H	0.156044	31 H	0.194826		
32 H	0.039421	32 H	0.018898	32 H	-0.068573	32 H	0.063190	32 H	0.045906	32 H	-0.051303		
33 C	-0.050554	33 C	-0.050068	33 C	-0.048193	33 C	-0.091425	33 C	-0.091497	33 C	-0.090317		
34 H	0.121942	34 H	0.138427	34 H	0.198070	34 H	0.145472	34 H	0.159194	34 H	0.229437		
35 H	0.038516	35 H	0.027118	35 H	-0.018390	35 H	0.054640	35 H	0.040696	35 H	-0.009491		
36 H	0.026251	36 H	0.009510	36 H	-0.068219	36 H	0.049244	36 H	0.030199	36 H	-0.047233		
37 H	0.016451	37 H	-0.003653	37 H	-0.097571	37 H	0.031888	37 H	0.009329	37 H	-0.083011		
38 H	0.116329	38 H	0.124935	38 H	0.156988	38 H	0.137490	38 H	0.150162	38 H	0.186899		
39 C	-0.149860	39 C	-0.138107	39 C	-0.066318	39 C	-0.179933	39 C	-0.171619	39 C	-0.111029		
40 H	0.028399	40 H	0.009251	40 H	-0.092576	40 H	0.046374	40 H	0.027768	40 H	-0.065037		
41 H	0.035139	41 H	0.021948	41 H	-0.054709	41 H	0.048903	41 H	0.033062	41 H	-0.022970		
42 C	-0.183681	42 C	-0.184911	42 C	-0.188709	42 C	-0.224974	42 C	-0.226641	42 C	-0.227342		
43 H	0.127557	43 H	0.130596	43 H	0.141355	43 H	0.146387	43 H	0.155594	43 H	0.166679		
44 H	0.140108	44 H	0.141862	44 H	0.150083	44 H	0.164915	44 H	0.177124	44 H	0.181599		
45 C	-0.167883	45 C	-0.150275	45 C	-0.078018	45 C	-0.207774	45 C	-0.200033	45 C	-0.130137		
46 H	0.118615	46 H	0.114921	46 H	0.107204	46 H	0.141877	46 H	0.147683	46 H	0.139374		
47 H	0.046067	47 H	0.011850	47 H	-0.125286	47 H	0.063586	47 H	0.041832	47 H	-0.095077		
48 C	-0.154625	48 C	-0.118363	48 C	0.000812	48 C	-0.202491	48 C	-0.183656	48 C	-0.035164		
49 H	0.051053	49 H	-0.028615	49 H	-0.377534	49 H	0.068552	49 H	0.028140	49 H	-0.375497		
50 H	0.121254	50 H	0.092660	50 H	0.005539	50 H	0.143290	50 H	0.139053	50 H	0.026614		
51 C	-0.305420	51 C	-0.151652	51 C	0.367248	51 C	-0.350045	51 C	-0.282757	51 C	0.348070		
52 H	0.128646	52 H	0.053409	52 H	-0.188094	52 H	0.147002	52 H	0.123123	52 H	-0.186980		
53 H	0.045110	53 H	-0.126024	53 H	-0.737354	53 H	0.061076	53 H	-0.022860	53 H	-0.764782		
54 F	-0.274331	54 F	-0.215519	54 F	0.042069	54 F	-0.299775	54 F	-0.268273	54 F	0.023724		
55 H	0.047319	55 H	0.032323	55 H	-0.029564	55 H	0.066306	55 H	0.051348	55 H	-0.019029		
56 H	0.114067	56 H	0.121879	56 H	0.152699	56 H	0.135584	56 H	0.144199	56 H	0.178390		
57 H	0.130839	57 H	0.151085	57 H	0.227333	57 H	0.152713	57 H	0.167661	57 H	0.253686		
58 H	0.069473	58 H	0.069535	58 H	0.069946	58 H	0.089061	58 H	0.082812	58 H	0.083290		
59 H	0.025468	59 H	-0.169911	59 H	-0.882489	59 H	0.045226	59 H	-0.052484	59 H	-0.905083		

Table S7. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S5) of Molecule 3 (Dihedral angle around 180°)

MOLECULE 3											
B3LYP						M062X					
FIELD = 0.012a.u.		FIELD = 0.018a.u.		FIELD = 0.04a.u.		FIELD = 0.012a.u.		FIELD = 0.018a.u.		FIELD = 0.04a.u.	
1 C	-0.058075	1 C	-0.035656	1 C	0.020379	1 C	-0.095262	1 C	-0.065725	1 C	0.004351
2 C	-0.106507	2 C	-0.096308	2 C	-0.072348	2 C	-0.134949	2 C	-0.122286	2 C	-0.099251
3 C	0.068375	3 C	0.087501	3 C	0.133815	3 C	0.029752	3 C	0.055083	3 C	0.117072
4 C	-0.107750	4 C	-0.098782	4 C	-0.078779	4 C	-0.135954	4 C	-0.124883	4 C	-0.105814
5 C	-0.056687	5 C	-0.035435	5 C	0.015291	5 C	-0.093697	5 C	-0.066246	5 C	-0.004643
6 H	0.178751	6 H	0.224247	6 H	0.316339	6 H	0.197470	6 H	0.253065	6 H	0.352812
7 H	0.120270	7 H	0.154668	7 H	0.225657	7 H	0.133343	7 H	0.179816	7 H	0.262167
8 H	0.076600	8 H	0.100063	8 H	0.149448	8 H	0.087389	8 H	0.124126	8 H	0.187510
9 H	0.149373	9 H	0.188060	9 H	0.267845	9 H	0.167026	9 H	0.216770	9 H	0.306028
10 C	0.062737	10 C	0.060711	10 C	0.059204	10 C	0.036788	10 C	0.030909	10 C	0.017884
11 C	-0.104148	11 C	-0.093564	11 C	-0.063078	11 C	-0.126323	11 C	-0.114008	11 C	-0.080050
12 C	-0.105571	12 C	-0.097576	12 C	-0.077730	12 C	-0.127964	12 C	-0.118936	12 C	-0.097810
13 C	-0.133367	13 C	-0.130985	13 C	-0.122968	13 C	-0.159646	13 C	-0.156663	13 C	-0.149297
14 H	0.152977	14 H	0.182086	14 H	0.247032	14 H	0.182790	14 H	0.213674	14 H	0.277911
15 C	-0.125777	15 C	-0.121907	15 C	-0.112047	15 C	-0.150232	15 C	-0.146196	15 C	-0.138038
16 H	0.079413	16 H	0.087369	16 H	0.108325	16 H	0.107928	16 H	0.118061	16 H	0.139114
17 C	0.124991	17 C	0.133151	17 C	0.153320	17 C	0.080329	17 C	0.089654	17 C	0.110069
18 H	0.094847	18 H	0.118984	18 H	0.173178	18 H	0.116636	18 H	0.147068	18 H	0.205404
19 H	0.028071	19 H	0.032300	19 H	0.043999	19 H	0.047221	19 H	0.058075	19 H	0.074147
20 C	-0.258315	20 C	-0.263178	20 C	-0.273206	20 C	-0.284515	20 C	-0.290054	20 C	-0.300868
21 C	-0.159110	21 C	-0.160796	21 C	-0.164746	21 C	-0.187356	21 C	-0.188993	21 C	-0.192141
22 C	-0.051829	22 C	-0.052740	22 C	-0.054137	22 C	-0.094455	22 C	-0.095704	22 C	-0.098024
23 C	-0.172580	23 C	-0.171700	23 C	-0.168812	23 C	-0.208031	23 C	-0.206975	23 C	-0.203328
24 C	-0.170369	24 C	-0.167797	24 C	-0.161520	24 C	-0.203034	24 C	-0.199733	24 C	-0.191883
25 H	0.111961	25 H	0.125842	25 H	0.157188	25 H	0.132245	25 H	0.147116	25 H	0.179895
26 C	-0.180825	26 C	-0.180246	26 C	-0.178356	26 C	-0.216242	26 C	-0.215473	26 C	-0.213555
27 H	0.050765	27 H	0.037384	27 H	0.006251	27 H	0.069836	27 H	0.054835	27 H	0.021115
28 H	0.147763	28 H	0.159268	28 H	0.185110	28 H	0.178647	28 H	0.187865	28 H	0.212101
29 C	-0.168776	29 C	-0.164464	29 C	-0.153224	29 C	-0.204359	29 C	-0.199560	29 C	-0.187872
30 H	0.041873	30 H	0.024967	30 H	-0.014691	30 H	0.060170	30 H	0.041657	30 H	-0.000659
31 H	0.099155	31 H	0.098454	31 H	0.096340	31 H	0.128822	31 H	0.126227	31 H	0.122148
32 C	-0.039607	32 C	-0.034153	32 C	-0.018361	32 C	-0.077610	32 C	-0.071118	32 C	-0.053753
33 H	0.060474	33 H	0.054234	33 H	0.039323	33 H	0.083365	33 H	0.077595	33 H	0.062753
34 H	0.118672	34 H	0.129809	34 H	0.153937	34 H	0.137861	34 H	0.149672	34 H	0.175118
35 H	0.019294	35 H	0.003797	35 H	-0.032288	35 H	0.033462	35 H	0.020070	35 H	-0.014647
36 H	0.108240	36 H	0.116860	36 H	0.134836	36 H	0.127145	36 H	0.136682	36 H	0.156182
37 H	0.025452	37 H	0.004435	37 H	-0.044715	37 H	0.046551	37 H	0.022819	37 H	-0.029610
38 C	-0.157320	38 C	-0.147456	38 C	-0.125446	38 C	-0.196765	38 C	-0.183456	38 C	-0.156926
39 H	0.060238	39 H	0.049661	39 H	0.022208	39 H	0.082003	39 H	0.070645	39 H	0.043895
40 H	0.112820	40 H	0.118591	40 H	0.127045	40 H	0.131119	40 H	0.137929	40 H	0.148001
41 C	-0.157103	41 C	-0.142144	41 C	-0.083124	41 C	-0.198581	41 C	-0.183222	41 C	-0.133294
42 H	0.081971	42 H	0.062355	42 H	0.006093	42 H	0.109865	42 H	0.086813	42 H	0.028710
43 H	0.023288	43 H	-0.029754	43 H	-0.202759	43 H	0.062345	43 H	0.006284	43 H	-0.156134
44 C	-0.108431	44 C	-0.020313	44 C	0.184333	44 C	-0.187155	44 C	-0.087798	44 C	0.136752
45 H	0.027566	45 H	-0.045447	45 H	-0.214170	45 H	0.080057	45 H	-0.009239	45 H	-0.190550
46 H	-0.067503	46 H	-0.216864	46 H	-0.561404	46 H	0.009865	46 H	-0.157042	46 H	-0.553261
47 C	-0.140766	47 C	-0.113046	47 C	-0.078488	47 C	-0.209247	47 C	-0.157565	47 C	-0.099189
48 H	0.134946	48 H	0.117079	48 H	0.093145	48 H	0.181633	48 H	0.147064	48 H	0.105878
49 H	0.066148	49 H	0.017005	49 H	-0.073409	49 H	0.121040	49 H	0.048883	49 H	-0.059574
50 C	-0.227779	50 C	-0.095259	50 C	0.184780	50 C	-0.352269	50 C	-0.174524	50 C	0.146142
51 H	0.056814	51 H	-0.030836	51 H	-0.226212	51 H	0.134316	51 H	0.019497	51 H	-0.211570
52 H	0.012895	52 H	-0.103278	52 H	-0.358610	52 H	0.095885	52 H	-0.057198	52 H	-0.370339
53 H	-0.094046	53 H	-0.297717	53 H	-0.718996	53 H	0.027906	53 H	-0.248524	53 H	-0.704427
54 C	-0.106497	54 C	-0.114535	54 C	-0.121921	54 C	-0.141032	54 C	-0.151931	54 C	-0.160383
55 H	0.098118	55 H	0.106537	55 H	0.126674	55 H	0.111523	55 H	0.122730	55 H	0.144805
56 H	0.134328	56 H	0.155146	56 H	0.202434	56 H	0.152846	56 H	0.176656	56 H	0.226279
57 H	0.098474	57 H	0.100328	57 H	0.105224	57 H	0.119818	57 H	0.120933	57 H	0.124639
58 H	0.054333	58 H	0.043009	58 H	0.016872	58 H	0.070770	58 H	0.058773	58 H	0.030713
59 Cl	0.176744	59 Cl	0.368033	59 Cl	0.799917	59 Cl	0.108909	59 Cl	0.346010	59 Cl	0.837295

Table S8. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S5) of Molecule 4 (Dihedral angle around 180°)

MOLECULE 4											
B3LYP						M062X					
FIELD = 0.016a.u.		FIELD = 0.024a.u.		FIELD = 0.044a.u.		FIELD = 0.016a.u.		FIELD = 0.024a.u.		FIELD = 0.036a.u.	
1 C	-0.078991	1 C	-0.054734	1 C	-0.004464	1 C	-0.097422	1 C	-0.078763	1 C	-0.141432
2 C	-0.117645	2 C	-0.105140	2 C	-0.071723	2 C	-0.140884	2 C	-0.131490	2 C	-0.219008
3 C	0.069216	3 C	0.090640	3 C	0.131802	3 C	0.041627	3 C	0.056259	3 C	-0.202944
4 C	-0.123742	4 C	-0.111809	4 C	-0.074317	4 C	-0.147049	4 C	-0.139853	4 C	-0.123237
5 C	-0.070560	5 C	-0.030873	5 C	0.085148	5 C	-0.085397	5 C	-0.050145	5 C	-0.113784
6 C	0.111578	6 C	0.133678	6 C	0.195549	6 C	0.062749	6 C	0.081311	6 C	-0.220528
7 H	0.090199	7 H	0.120342	7 H	0.179565	7 H	0.128421	7 H	0.147553	7 H	0.225168
8 H	0.021063	8 H	0.027642	8 H	0.035269	8 H	0.052544	8 H	0.045809	8 H	0.103415
9 H	0.137834	9 H	0.192465	9 H	0.301797	9 H	0.171161	9 H	0.216110	9 H	0.316977
10 H	0.203187	10 H	0.275451	10 H	0.414843	10 H	0.240709	10 H	0.302943	10 H	0.416069
11 C	0.062178	11 C	0.059389	11 C	0.055464	11 C	0.033835	11 C	0.031006	11 C	-0.006886
12 C	-0.107913	12 C	-0.096136	12 C	-0.062628	12 C	-0.126231	12 C	-0.116112	12 C	-0.142184
13 C	-0.105716	13 C	-0.096810	13 C	-0.078989	13 C	-0.124652	13 C	-0.117364	13 C	-0.156746
14 C	-0.133558	14 C	-0.131195	14 C	-0.122945	14 C	-0.156501	14 C	-0.156561	14 C	-0.145073
15 H	0.147065	15 H	0.185203	15 H	0.267081	15 H	0.182761	15 H	0.217563	15 H	0.279469
16 C	-0.127993	16 C	-0.124166	16 C	-0.114413	16 C	-0.150851	16 C	-0.147988	16 C	-0.148158
17 H	0.075473	17 H	0.080437	17 H	0.086601	17 H	0.110294	17 H	0.111425	17 H	0.128036
18 C	0.118502	18 C	0.126319	18 C	0.141773	18 C	0.079352	18 C	0.084730	18 C	0.042577
19 H	0.090788	19 H	0.121875	19 H	0.186073	19 H	0.125914	19 H	0.149094	19 H	0.215581
20 H	0.003649	20 H	-0.007323	20 H	-0.045861	20 H	0.037501	20 H	0.016600	20 H	0.028564
21 C	-0.252955	21 C	-0.257882	21 C	-0.268020	21 C	-0.280897	21 C	-0.286074	21 C	-0.294318
22 C	-0.159553	22 C	-0.159516	22 C	-0.157366	22 C	-0.189027	22 C	-0.188294	22 C	-0.192979
23 C	-0.042639	23 C	-0.037931	23 C	-0.025174	23 C	-0.081477	23 C	-0.076410	23 C	-0.069847
24 C	-0.182441	24 C	-0.186441	24 C	-0.194252	24 C	-0.219879	24 C	-0.224083	24 C	-0.231906
25 C	-0.164121	25 C	-0.158618	25 C	-0.142404	25 C	-0.200690	25 C	-0.195001	25 C	-0.185863
26 H	0.027647	26 H	0.009460	26 H	-0.039804	26 H	0.047853	26 H	0.026672	26 H	0.004766
27 C	-0.179551	27 C	-0.178512	27 C	-0.174655	27 C	-0.213097	27 C	-0.212850	27 C	-0.207435
28 H	0.133000	28 H	0.149292	28 H	0.190632	28 H	0.150669	28 H	0.169635	28 H	0.188577
29 H	0.124868	29 H	0.138110	29 H	0.172106	29 H	0.151254	29 H	0.167219	29 H	0.180428
30 C	-0.161825	30 C	-0.152257	30 C	-0.125211	30 C	-0.192348	30 C	-0.181819	30 C	-0.163836
31 H	0.120090	31 H	0.130513	31 H	0.157958	31 H	0.137680	31 H	0.150722	31 H	0.161175
32 H	0.053147	32 H	0.028644	32 H	-0.032599	32 H	0.077299	32 H	0.055161	32 H	0.006691
33 C	-0.050050	33 C	-0.048891	33 C	-0.045950	33 C	-0.090676	33 C	-0.090128	33 C	-0.085277
34 H	0.110786	34 H	0.129459	34 H	0.171269	34 H	0.133924	34 H	0.150895	34 H	0.185488
35 H	0.045009	35 H	0.030295	35 H	-0.007705	35 H	0.061373	35 H	0.044696	35 H	0.026066
36 H	0.032580	36 H	0.009171	36 H	-0.053660	36 H	0.055703	36 H	0.030611	36 H	-0.003491
37 H	0.027326	37 H	0.001864	37 H	-0.066412	37 H	0.043052	37 H	0.015719	37 H	-0.020553
38 H	0.108763	38 H	0.117646	38 H	0.141530	38 H	0.129638	38 H	0.141797	38 H	0.146879
39 C	-0.151910	39 C	-0.135262	39 C	-0.085952	39 C	-0.182421	39 C	-0.168241	39 C	-0.127342
40 H	0.033742	40 H	0.006765	40 H	-0.070878	40 H	0.052063	40 H	0.025753	40 H	-0.015380
41 H	0.043074	41 H	0.027003	41 H	-0.022124	41 H	0.057057	41 H	0.039599	41 H	0.030592
42 C	-0.181510	42 C	-0.182273	42 C	-0.182859	42 C	-0.222496	42 C	-0.223223	42 C	-0.204549
43 H	0.123075	43 H	0.125179	43 H	0.133194	43 H	0.141677	43 H	0.148493	43 H	0.137828
44 H	0.130268	44 H	0.127587	44 H	0.128166	44 H	0.154879	44 H	0.160127	44 H	0.131925
45 C	-0.166406	45 C	-0.136181	45 C	-0.065026	45 C	-0.206181	45 C	-0.184116	45 C	-0.109011
46 H	0.105735	46 H	0.091320	46 H	0.070334	46 H	0.128575	46 H	0.121893	46 H	0.107804
47 H	0.047993	47 H	-0.006780	47 H	-0.136416	47 H	0.065658	47 H	0.022188	47 H	0.002191
48 C	-0.155441	48 C	-0.103971	48 C	-0.018341	48 C	-0.203536	48 C	-0.159934	48 C	0.015693
49 H	0.063139	49 H	-0.047168	49 H	-0.317631	49 H	0.081124	49 H	-0.002265	49 H	-0.038794
50 H	0.118587	50 H	0.072722	50 H	-0.003635	50 H	0.140507	50 H	0.112245	50 H	0.058310
51 C	-0.306284	51 C	-0.070689	51 C	0.412085	51 C	-0.350900	51 C	-0.177469	51 C	0.115134
52 H	0.116835	52 H	-0.014899	52 H	-0.276071	52 H	0.134815	52 H	0.041361	52 H	0.004321
53 H	0.049009	53 H	-0.210624	53 H	-0.764440	53 H	0.065070	53 H	-0.132534	53 H	-0.056426
54 C	0.096138	54 C	0.207582	54 C	0.468486	54 C	0.107612	54 C	0.183071	54 C	0.223037
55 N	-0.225356	55 N	-0.108177	55 N	0.179280	55 N	-0.228309	55 N	-0.127335	55 N	-0.275451
56 H	0.123157	56 H	0.147106	56 H	0.200440	56 H	0.144928	56 H	0.165668	56 H	0.212018
57 H	0.073179	57 H	0.072282	57 H	0.065977	57 H	0.092597	57 H	0.087361	57 H	0.096935
58 H	0.060545	58 H	0.043240	58 H	-0.000808	58 H	0.079777	58 H	0.062634	58 H	0.031860
59 H	0.112746	59 H	0.123085	59 H	0.148717	59 H	0.134299	59 H	0.145481	59 H	0.160154
60 H	0.034986	60 H	-0.247510	60 H	-0.868407	60 H	0.054969	60 H	-0.161353	60 H	-0.081289

Table S9. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S10) of Molecule 1 (Dihedral Angle around 290°)

MOLECULE 1											
B3LYP						M062X					
FIELD = 0.012a.u.		FIELD = 0.02a.u.		FIELD = 0.04a.u.		FIELD = 0.012a.u.		FIELD = 0.02a.u.		FIELD = 0.04a.u.	
1 C	-0.088825	1 C	-0.069671	1 C	0.040799	1 C	-0.124142	1 C	-0.112991	1 C	0.016450
2 C	-0.115000	2 C	-0.102311	2 C	-0.062633	2 C	-0.136218	2 C	-0.130612	2 C	-0.093953
3 C	0.058604	3 C	0.078828	3 C	0.152832	3 C	0.031708	3 C	0.040290	3 C	0.136104
4 C	-0.114312	4 C	-0.101296	4 C	-0.048650	4 C	-0.135632	4 C	-0.129186	4 C	-0.072115
5 C	-0.088202	5 C	-0.073400	5 C	-0.023347	5 C	-0.124008	5 C	-0.116756	5 C	-0.067090
6 H	0.148091	6 H	0.220872	6 H	0.399959	6 H	0.183739	6 H	0.239368	6 H	0.432567
7 H	0.098852	7 H	0.140909	7 H	0.258381	7 H	0.131109	7 H	0.156931	7 H	0.293795
8 H	0.043575	8 H	0.056540	8 H	0.130708	8 H	0.075050	8 H	0.066946	8 H	0.167858
9 H	0.099982	9 H	0.148857	9 H	0.285626	9 H	0.135473	9 H	0.165154	9 H	0.322363
10 C	0.062217	10 C	0.060275	10 C	0.054325	10 C	0.033706	10 C	0.032493	10 C	0.011761
11 C	-0.108327	11 C	-0.097120	11 C	-0.061240	11 C	-0.126471	11 C	-0.118614	11 C	-0.079536
12 C	-0.109303	12 C	-0.098368	12 C	-0.058297	12 C	-0.127568	12 C	-0.121008	12 C	-0.076181
13 C	-0.136432	13 C	-0.136065	13 C	-0.128941	13 C	-0.159395	13 C	-0.162651	13 C	-0.156001
14 H	0.111613	14 H	0.139453	14 H	0.211187	14 H	0.146440	14 H	0.168817	14 H	0.241943
15 C	-0.143964	15 C	-0.141921	15 C	-0.131610	15 C	-0.167999	15 C	-0.169198	15 C	-0.159828
16 H	0.104568	16 H	0.130573	16 H	0.202269	16 H	0.139648	16 H	0.158939	16 H	0.233431
17 C	0.125587	17 C	0.128511	17 C	0.145240	17 C	0.080391	17 C	0.078513	17 C	0.097590
18 H	0.053806	18 H	0.058951	18 H	0.091157	18 H	0.087135	18 H	0.080346	18 H	0.120760
19 H	0.052777	19 H	0.060081	19 H	0.098915	19 H	0.087194	19 H	0.081541	19 H	0.129809
20 C	-0.243115	20 C	-0.244729	20 C	-0.249875	20 C	-0.268141	20 C	-0.268656	20 C	-0.275279
21 C	-0.161582	21 C	-0.161010	21 C	-0.163271	21 C	-0.194199	21 C	-0.190902	21 C	-0.194201
22 C	-0.038611	22 C	-0.036322	22 C	-0.031247	22 C	-0.077527	22 C	-0.074954	22 C	-0.070356
23 C	-0.177623	23 C	-0.178599	23 C	-0.180381	23 C	-0.206608	23 C	-0.208359	23 C	-0.210446
24 C	-0.168703	24 C	-0.163534	24 C	-0.150638	24 C	-0.201294	24 C	-0.195130	24 C	-0.180855
25 H	0.065924	25 H	0.065635	25 H	0.066614	25 H	0.084481	25 H	0.083194	25 H	0.085177
26 C	-0.185633	26 C	-0.188179	26 C	-0.190915	26 C	-0.219425	26 C	-0.224007	26 C	-0.226189
27 H	0.090015	27 H	0.093267	27 H	0.097882	27 H	0.107632	27 H	0.112988	27 H	0.115235
28 H	0.154980	28 H	0.169225	28 H	0.186433	28 H	0.174446	28 H	0.200182	28 H	0.210390
29 C	-0.163186	29 C	-0.154237	29 C	-0.127243	29 C	-0.196297	29 C	-0.186790	29 C	-0.159260
30 H	0.076806	30 H	0.071491	30 H	0.056536	30 H	0.094406	30 H	0.089782	30 H	0.073424
31 H	0.052279	31 H	0.031945	31 H	-0.022190	31 H	0.075623	31 H	0.055274	31 H	-0.000472
32 C	-0.048710	32 C	-0.047325	32 C	-0.041222	32 C	-0.087478	32 C	-0.086548	32 C	-0.078653
33 H	0.105513	33 H	0.116809	33 H	0.140074	33 H	0.131196	33 H	0.144574	33 H	0.166546
34 H	0.082498	34 H	0.085097	34 H	0.091122	34 H	0.100076	34 H	0.102446	34 H	0.109444
35 H	0.026216	35 H	-0.004338	35 H	-0.071931	35 H	0.046404	35 H	0.008610	35 H	-0.054912
36 H	0.066177	36 H	0.059120	36 H	0.042085	36 H	0.083741	36 H	0.075245	36 H	0.060363
37 H	0.072037	37 H	0.067198	37 H	0.050273	37 H	0.091233	37 H	0.089183	37 H	0.068321
38 C	-0.165666	38 C	-0.160186	38 C	-0.140173	38 C	-0.199654	38 C	-0.198082	38 C	-0.172446
39 H	0.101564	39 H	0.109610	39 H	0.120163	39 H	0.122583	39 H	0.134208	39 H	0.142912
40 H	0.078784	40 H	0.076680	40 H	0.069893	40 H	0.094350	40 H	0.091351	40 H	0.087769
41 C	-0.167926	41 C	-0.158419	41 C	-0.110146	41 C	-0.206163	41 C	-0.197711	41 C	-0.159998
42 H	0.058366	42 H	0.025694	42 H	-0.100034	42 H	0.074475	42 H	0.047651	42 H	-0.065277
43 H	0.083456	43 H	0.061823	43 H	-0.029237	43 H	0.106473	43 H	0.096607	43 H	0.001689
44 C	-0.159444	44 C	-0.114966	44 C	0.046728	44 C	-0.199146	44 C	-0.173816	44 C	0.005776
45 H	0.106547	45 H	0.089655	45 H	0.026477	45 H	0.126478	45 H	0.126190	45 H	0.050005
46 H	0.028202	46 H	-0.067439	46 H	-0.396612	46 H	0.048597	46 H	-0.018334	46 H	-0.381877
47 C	-0.158438	47 C	-0.108400	47 C	0.025881	47 C	-0.206654	47 C	-0.175582	47 C	0.004328
48 H	0.134910	48 H	0.116256	48 H	0.055471	48 H	0.155291	48 H	0.160117	48 H	0.069778
49 H	0.056328	49 H	-0.047001	49 H	-0.395090	49 H	0.076097	49 H	0.013853	49 H	-0.393132
50 C	-0.307983	50 C	-0.171605	50 C	0.236514	50 C	-0.353213	50 C	-0.283260	50 C	0.197111
51 H	0.073972	51 H	-0.060059	51 H	-0.502096	51 H	0.094971	51 H	0.022555	51 H	-0.506017
52 H	0.121453	52 H	0.051882	52 H	-0.155106	52 H	0.139704	52 H	0.113613	52 H	-0.141776
53 H	0.042799	53 H	-0.170031	53 H	-0.779995	53 H	0.058365	53 H	-0.072130	53 H	-0.767008
54 C	-0.073749	54 C	-0.031775	54 C	0.165623	54 C	-0.109126	54 C	-0.081077	54 C	0.172767
55 H	0.151046	55 H	0.231702	55 H	0.420539	55 H	0.186774	55 H	0.247598	55 H	0.455151
56 H	0.077205	56 H	0.078224	56 H	0.090610	56 H	0.098436	56 H	0.093710	56 H	0.110173
57 H	0.117427	57 H	0.133447	57 H	0.179220	57 H	0.144394	57 H	0.156530	57 H	0.205207
58 H	0.047834	58 H	0.033623	58 H	0.008444	58 H	0.069424	58 H	0.048780	58 H	0.026555
59 H	0.092722	59 H	0.096072	59 H	0.104142	59 H	0.109112	59 H	0.112776	59 H	0.120307

Table S10. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S10) of Molecule 2 (Dihedral Angle around 290°)

MOLECULE 2					
B3LYP			M062X		
FIELD = 0.012a.u.	FIELD = 0.02a.u.	FIELD = 0.04a.u.	FIELD = 0.012a.u.	FIELD = 0.02a.u.	FIELD = 0.04a.u.
1 C -0.146825	1 C -0.120556	1 C -0.028746	1 C -0.178107	1 C -0.162030	1 C -0.052863
2 C -0.110845	2 C -0.099275	2 C -0.066698	2 C -0.131032	2 C -0.124887	2 C -0.091821
3 C 0.053497	3 C 0.075294	3 C 0.152349	3 C 0.025850	3 C 0.036681	3 C 0.138103
4 C -0.111950	4 C -0.101180	4 C -0.072287	4 C -0.132463	4 C -0.127003	4 C -0.097327
5 C -0.145346	5 C -0.119756	5 C -0.034926	5 C -0.176914	5 C -0.161402	5 C -0.062415
6 C 0.412470	6 C 0.452001	6 C 0.580616	6 C 0.419738	6 C 0.449655	6 C 0.611865
7 H 0.152517	7 H 0.209343	7 H 0.353742	7 H 0.190509	7 H 0.231083	7 H 0.389926
8 H 0.097889	8 H 0.135031	8 H 0.233864	8 H 0.130831	8 H 0.152861	8 H 0.271233
9 H 0.065045	9 H 0.092795	9 H 0.169758	9 H 0.097775	9 H 0.108253	9 H 0.208747
10 H 0.131270	10 H 0.182182	10 H 0.314403	10 H 0.169360	10 H 0.203220	10 H 0.352432
11 C 0.063542	11 C 0.061202	11 C 0.057437	11 C 0.035372	11 C 0.033390	11 C 0.013262
12 C -0.109164	12 C -0.097770	12 C -0.053495	12 C -0.127029	12 C -0.118932	12 C -0.067270
13 C -0.109650	13 C -0.099501	13 C -0.065638	13 C -0.128056	13 C -0.121918	13 C -0.083334
14 C -0.140469	14 C -0.138066	14 C -0.127059	14 C -0.164024	14 C -0.165765	14 C -0.155061
15 H 0.135966	15 H 0.167409	15 H 0.256443	15 H 0.171076	15 H 0.197564	15 H 0.288067
16 C -0.143584	16 C -0.139102	16 C -0.124322	16 C -0.165039	16 C -0.163297	16 C -0.150218
17 H 0.079118	17 H 0.093093	17 H 0.138090	17 H 0.114092	17 H 0.120545	17 H 0.170149
18 C 0.128836	18 C 0.134309	18 C 0.153224	18 C 0.085404	18 C 0.086363	18 C 0.107917
19 H 0.082079	19 H 0.104531	19 H 0.170938	19 H 0.115893	19 H 0.128491	19 H 0.202849
20 H 0.027765	20 H 0.034260	20 H 0.058010	20 H 0.060095	20 H 0.052793	20 H 0.087214
21 C -0.244777	21 C -0.247810	21 C -0.255745	21 C -0.271619	21 C -0.273382	21 C -0.282805
22 C -0.171104	22 C -0.173626	22 C -0.181539	22 C -0.202902	22 C -0.203276	22 C -0.213742
23 C -0.035554	23 C -0.033792	23 C -0.028834	23 C -0.074065	23 C -0.071033	23 C -0.065785
24 C -0.170378	24 C -0.168210	24 C -0.161495	24 C -0.201452	24 C -0.199070	24 C -0.192531
25 C -0.178795	25 C -0.180271	25 C -0.184468	25 C -0.209284	25 C -0.211280	25 C -0.215608
26 H 0.033122	26 H 0.024956	26 H 0.001507	26 H 0.052044	26 H 0.038965	26 H 0.018034
27 C -0.165826	27 C -0.160490	27 C -0.143608	27 C -0.197440	27 C -0.191868	27 C -0.173295
28 H 0.119255	28 H 0.123825	28 H 0.136443	28 H 0.132237	28 H 0.141911	28 H 0.151175
29 H 0.058795	29 H 0.050050	29 H 0.023901	29 H 0.082615	29 H 0.073541	29 H 0.046649
30 C -0.178572	30 C -0.177144	30 C -0.172414	30 C -0.210965	30 C -0.210274	30 C -0.204239
31 H 0.142075	31 H 0.143006	31 H 0.144196	31 H 0.154577	31 H 0.163667	31 H 0.158277
32 H 0.116044	32 H 0.122989	32 H 0.143461	32 H 0.140965	32 H 0.152017	32 H 0.169087
33 C -0.053178	33 C -0.052576	33 C -0.050556	33 C -0.092997	33 C -0.093481	33 C -0.090930
34 H 0.044780	34 H 0.036083	34 H 0.011237	34 H 0.065670	34 H 0.052113	34 H 0.030269
35 H 0.035482	35 H 0.021915	35 H -0.018813	35 H 0.051625	35 H 0.034489	35 H -0.004284
36 H 0.098252	36 H 0.101918	36 H 0.112760	36 H 0.123790	36 H 0.128892	36 H 0.138165
37 H 0.045151	37 H 0.037097	37 H 0.013290	37 H 0.061153	37 H 0.049590	37 H 0.027986
38 H 0.106731	38 H 0.109437	38 H 0.116710	38 H 0.127493	38 H 0.135982	38 H 0.138376
39 C -0.162417	39 C -0.155508	39 C -0.134298	39 C -0.195036	39 C -0.190840	39 C -0.166276
40 H 0.093234	40 H 0.093637	40 H 0.093540	40 H 0.113879	40 H 0.116790	40 H 0.114590
41 H 0.048326	41 H 0.039487	41 H 0.013282	41 H 0.062389	41 H 0.049869	41 H 0.027306
42 C -0.172932	42 C -0.169614	42 C -0.155905	42 C -0.212148	42 C -0.208968	42 C -0.191249
43 H 0.064878	43 H 0.046971	43 H -0.009079	43 H 0.081217	43 H 0.066432	43 H 0.006409
44 H 0.119080	44 H 0.111622	44 H 0.086616	44 H 0.143399	44 H 0.146731	44 H 0.111274
45 C -0.163602	45 C -0.138980	45 C -0.056465	45 C -0.203831	45 C -0.188962	45 C -0.115237
46 H 0.051383	46 H 0.012555	46 H -0.113160	46 H 0.072533	46 H 0.045060	46 H -0.071490
47 H 0.104049	47 H 0.088030	47 H 0.041738	47 H 0.123873	47 H 0.119127	47 H 0.068865
48 C -0.153447	48 C -0.107692	48 C 0.012921	48 C -0.201343	48 C -0.170134	48 C -0.023860
49 H 0.112898	49 H 0.067355	49 H -0.063635	49 H 0.132715	49 H 0.111432	49 H -0.044382
50 H 0.057832	50 H -0.030163	50 H -0.337190	50 H 0.077801	50 H 0.024189	50 H -0.313563
51 C -0.305815	51 C -0.119416	51 C 0.406654	51 C -0.350581	51 C -0.243308	51 C 0.380315
52 H 0.060699	52 H -0.125466	52 H -0.658419	52 H 0.076966	52 H -0.036021	52 H -0.662024
53 H 0.112008	53 H -0.000978	53 H -0.323515	53 H 0.130075	53 H 0.069771	53 H -0.330501
54 F -0.281430	54 F -0.214877	54 F 0.007837	54 F -0.306369	54 F -0.264523	54 F -0.022471
55 H 0.111033	55 H 0.120438	55 H 0.148829	55 H 0.130447	55 H 0.140783	55 H 0.168963
56 H 0.055727	56 H 0.054659	56 H 0.053630	56 H 0.078599	56 H 0.071774	56 H 0.074525
57 H 0.137281	57 H 0.158957	57 H 0.223197	57 H 0.165248	57 H 0.183425	57 H 0.250639
58 H 0.064973	58 H 0.064935	58 H 0.067317	58 H 0.082875	58 H 0.076294	58 H 0.082922
59 H 0.032577	59 H -0.199549	59 H -0.875629	59 H 0.052518	59 H -0.092089	59 H -0.861009

Table S11. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S10) of Molecule 3 (Dihedral Angle around 290°)

MOLECULE 3											
B3LYP						M062X					
FIELD = 0.012a.u.		FIELD = 0.024a.u.		FIELD = 0.036a.u.		FIELD = 0.012a.u.		FIELD = 0.024a.u.		FIELD = 0.036a.u.	
1 C	-0.068710	1 C	-0.020191	1 C	0.038726	1 C	-0.095029	1 C	-0.046289	1 C	0.027523
2 C	-0.112809	2 C	-0.093255	2 C	-0.071220	2 C	-0.135030	2 C	-0.118542	2 C	-0.099351
3 C	0.058715	3 C	0.094813	3 C	0.134614	3 C	0.031853	3 C	0.065301	3 C	0.116850
4 C	-0.111841	4 C	-0.093496	4 C	-0.074790	4 C	-0.134366	4 C	-0.118827	4 C	-0.101926
5 C	-0.069631	5 C	-0.029889	5 C	0.012464	5 C	-0.096473	5 C	-0.058688	5 C	-0.008843
6 H	0.160686	6 H	0.261648	6 H	0.348209	6 H	0.197572	6 H	0.293406	6 H	0.383245
7 H	0.110457	7 H	0.183983	7 H	0.250099	7 H	0.143615	7 H	0.213479	7 H	0.285651
8 H	0.053406	8 H	0.086333	8 H	0.120154	8 H	0.085941	8 H	0.114089	8 H	0.157591
9 H	0.112712	9 H	0.180481	9 H	0.242823	9 H	0.149592	9 H	0.212806	9 H	0.281340
10 C	0.062788	10 C	0.059286	10 C	0.057222	10 C	0.034456	10 C	0.027896	10 C	0.017262
11 C	-0.109332	11 C	-0.091271	11 C	-0.070063	11 C	-0.127447	11 C	-0.110257	11 C	-0.088099
12 C	-0.109837	12 C	-0.092355	12 C	-0.072173	12 C	-0.128147	12 C	-0.112123	12 C	-0.090991
13 C	-0.135887	13 C	-0.131687	13 C	-0.126574	13 C	-0.158884	13 C	-0.157360	13 C	-0.153333
14 H	0.115238	14 H	0.160102	14 H	0.203322	14 H	0.150123	14 H	0.192522	14 H	0.234325
15 C	-0.141944	15 C	-0.134557	15 C	-0.126609	15 C	-0.166028	15 C	-0.161058	15 C	-0.154359
16 H	0.096716	16 H	0.130144	16 H	0.164032	16 H	0.131786	16 H	0.162368	16 H	0.195464
17 C	0.125520	17 C	0.133459	17 C	0.142899	17 C	0.080528	17 C	0.085894	17 C	0.095374
18 H	0.065941	18 H	0.090783	18 H	0.116770	18 H	0.099643	18 H	0.120020	18 H	0.147376
19 H	0.053947	19 H	0.072978	19 H	0.093644	19 H	0.088601	19 H	0.102594	19 H	0.124977
20 C	-0.245571	20 C	-0.250375	20 C	-0.254464	20 C	-0.271075	20 C	-0.275859	20 C	-0.280353
21 C	-0.165956	21 C	-0.170465	21 C	-0.175392	21 C	-0.198964	21 C	-0.202555	21 C	-0.207645
22 C	-0.040018	22 C	-0.037694	22 C	-0.035565	22 C	-0.078718	22 C	-0.076303	22 C	-0.074085
23 C	-0.176859	23 C	-0.177551	23 C	-0.178009	23 C	-0.205857	23 C	-0.207216	23 C	-0.207768
24 C	-0.171197	24 C	-0.166245	24 C	-0.161357	24 C	-0.204253	24 C	-0.198645	24 C	-0.193141
25 H	0.065535	25 H	0.065173	25 H	0.065035	25 H	0.084118	25 H	0.083410	25 H	0.083383
26 C	-0.183858	26 C	-0.184240	26 C	-0.184291	26 C	-0.217340	26 C	-0.218707	26 C	-0.218471
27 H	0.091421	27 H	0.094337	27 H	0.097180	27 H	0.109064	27 H	0.112844	27 H	0.114573
28 H	0.150080	28 H	0.159488	28 H	0.167254	28 H	0.169375	28 H	0.184106	28 H	0.190243
29 C	-0.165393	29 C	-0.153282	29 C	-0.140148	29 C	-0.198560	29 C	-0.185671	29 C	-0.171581
30 H	0.081529	30 H	0.076342	30 H	0.071186	30 H	0.099288	30 H	0.094322	30 H	0.088395
31 H	0.064112	31 H	0.044040	31 H	0.023506	31 H	0.087877	31 H	0.067718	31 H	0.046302
32 C	-0.048328	32 C	-0.044710	32 C	-0.040341	32 C	-0.087320	32 C	-0.083627	32 C	-0.078405
33 H	0.095994	33 H	0.100915	33 H	0.105369	33 H	0.121357	33 H	0.127167	33 H	0.130653
34 H	0.078980	34 H	0.079450	34 H	0.079672	34 H	0.096439	34 H	0.097041	34 H	0.097490
35 H	0.031150	35 H	-0.004891	35 H	-0.040405	35 H	0.051471	35 H	0.011700	35 H	-0.023679
36 H	0.065770	36 H	0.055617	36 H	0.045206	36 H	0.083271	36 H	0.072689	36 H	0.062692
37 H	0.073676	37 H	0.063658	37 H	0.053609	37 H	0.092966	37 H	0.083782	37 H	0.071889
38 C	-0.164448	38 C	-0.150465	38 C	-0.136294	38 C	-0.198054	38 C	-0.185282	38 C	-0.168747
39 H	0.092369	39 H	0.091970	39 H	0.090144	39 H	0.113056	39 H	0.114260	39 H	0.111359
40 H	0.076483	40 H	0.072468	40 H	0.067253	40 H	0.091934	40 H	0.088519	40 H	0.084536
41 C	-0.168537	41 C	-0.154841	41 C	-0.134796	41 C	-0.207160	41 C	-0.192540	41 C	-0.175397
42 H	0.066660	42 H	0.020840	42 H	-0.034383	42 H	0.083154	42 H	0.040189	42 H	-0.011952
43 H	0.086544	43 H	0.043873	43 H	-0.006026	43 H	0.109743	43 H	0.072512	43 H	0.021452
44 C	-0.159288	44 C	-0.068227	44 C	0.037045	44 C	-0.198808	44 C	-0.128319	44 C	-0.015075
45 H	0.097850	45 H	0.042838	45 H	-0.011107	45 H	0.117486	45 H	0.070845	45 H	0.017666
46 H	0.029860	46 H	-0.139626	46 H	-0.335207	46 H	0.050321	46 H	-0.090119	46 H	-0.306824
47 C	-0.157542	47 C	-0.070641	47 C	-0.005544	47 C	-0.205988	47 C	-0.113378	47 C	-0.034361
48 H	0.132193	48 H	0.074864	48 H	0.030843	48 H	0.152559	48 H	0.100420	48 H	0.046315
49 H	0.065002	49 H	-0.115758	49 H	-0.306098	49 H	0.085117	49 H	-0.083280	49 H	-0.287229
50 C	-0.307767	50 C	0.012657	50 C	0.318308	50 C	-0.352751	50 C	-0.045920	50 C	0.289197
51 H	0.069473	51 H	-0.246995	51 H	-0.575112	51 H	0.090373	51 H	-0.203978	51 H	-0.576943
52 H	0.111053	52 H	-0.088473	52 H	-0.278113	52 H	0.129014	52 H	-0.055714	52 H	-0.278482
53 H	0.044144	53 H	-0.383399	53 H	-0.777820	53 H	0.059788	53 H	-0.361677	53 H	-0.771198
54 C	-0.100874	54 C	-0.118299	54 C	-0.125574	54 C	-0.139618	54 C	-0.156443	54 C	-0.166590
55 H	0.079146	55 H	0.085910	55 H	0.093845	55 H	0.100368	55 H	0.104845	55 H	0.113337
56 H	0.131536	56 H	0.169249	56 H	0.206390	56 H	0.158905	56 H	0.195581	56 H	0.232911
57 H	0.061458	57 H	0.056926	57 H	0.053671	57 H	0.083506	57 H	0.076320	57 H	0.073261
58 H	0.095169	58 H	0.101612	58 H	0.108312	58 H	0.111549	58 H	0.118194	58 H	0.123494
59 Cl	0.062315	59 Cl	0.446641	59 Cl	0.838668	59 Cl	0.080058	59 Cl	0.441540	59 Cl	0.877804

Table S12. Mulliken Charge Distribution on the Atoms (Along with Their Label Number as per Figure S10) of Molecule 4 (Dihedral Angle around 290°)

MOLECULE 4					
B3LYP			M062X		
FIELD = 0.014a.u.	FIELD = 0.022a.u.	FIELD = 0.04a.u.	FIELD = 0.014a.u.	FIELD = 0.022a.u.	FIELD = 0.04a.u.
1 C -0.078380	1 C -0.051104	1 C 0.002881	1 C -0.096478	1 C -0.074542	1 C -0.008981
2 C -0.119425	2 C -0.108166	2 C -0.083978	2 C -0.142646	2 C -0.134762	2 C -0.113464
3 C 0.070526	3 C 0.093676	3 C 0.139755	3 C 0.042999	3 C 0.059839	3 C 0.119566
4 C -0.123440	4 C -0.111546	4 C -0.082569	4 C -0.146907	4 C -0.139563	4 C -0.115309
5 C -0.073357	5 C -0.034451	5 C 0.066507	5 C -0.088861	5 C -0.053839	5 C 0.076517
6 C 0.110671	6 C 0.135023	6 C 0.194270	6 C 0.061846	6 C 0.082907	6 C 0.144281
7 H 0.105179	7 H 0.146113	7 H 0.219320	7 H 0.143402	7 H 0.173692	7 H 0.258574
8 H 0.035444	8 H 0.052934	8 H 0.080604	8 H 0.067306	8 H 0.071362	8 H 0.115958
9 H 0.126387	9 H 0.178688	9 H 0.274074	9 H 0.159600	9 H 0.203214	9 H 0.308069
10 H 0.188336	10 H 0.260858	10 H 0.389005	10 H 0.226076	10 H 0.289434	10 H 0.422659
11 C 0.060364	11 C 0.057646	11 C 0.053398	11 C 0.031912	11 C 0.028706	11 C 0.016479
12 C -0.107770	12 C -0.096211	12 C -0.069442	12 C -0.125583	12 C -0.115723	12 C -0.086190
13 C -0.106081	13 C -0.095069	13 C -0.073804	13 C -0.124065	13 C -0.115297	13 C -0.093313
14 C -0.138572	14 C -0.136170	14 C -0.132366	14 C -0.162036	14 C -0.162682	14 C -0.158524
15 H 0.127594	15 H 0.159468	15 H 0.221818	15 H 0.162948	15 H 0.191949	15 H 0.254150
16 C -0.146997	16 C -0.143726	16 C -0.138692	16 C -0.168771	16 C -0.167735	16 C -0.162924
17 H 0.097129	17 H 0.115936	17 H 0.150559	17 H 0.132041	17 H 0.146892	17 H 0.182264
18 C 0.129855	18 C 0.135049	18 C 0.143182	18 C 0.086628	18 C 0.088649	18 C 0.097754
19 H 0.077568	19 H 0.097903	19 H 0.134633	19 H 0.111154	19 H 0.125054	19 H 0.165962
20 H 0.031421	20 H 0.033910	20 H 0.029517	20 H 0.063879	20 H 0.057044	20 H 0.058172
21 C -0.243458	21 C -0.245715	21 C -0.248441	21 C -0.270301	21 C -0.271815	21 C -0.274944
22 C -0.169538	22 C -0.169882	22 C -0.168740	22 C -0.201179	22 C -0.200103	22 C -0.199859
23 C -0.034440	23 C -0.030397	23 C -0.020067	23 C -0.072921	23 C -0.067807	23 C -0.056493
24 C -0.169419	24 C -0.165468	24 C -0.155435	24 C -0.200477	24 C -0.196328	24 C -0.186198
25 C -0.179227	25 C -0.180864	25 C -0.183652	25 C -0.209712	25 C -0.212102	25 C -0.215836
26 H 0.031234	26 H 0.016314	26 H -0.021266	26 H 0.050079	26 H 0.031544	26 H -0.005310
27 C -0.164792	27 C -0.156460	27 C -0.136930	27 C -0.196306	27 C -0.187530	27 C -0.165911
28 H 0.119600	28 H 0.127216	28 H 0.147523	28 H 0.132740	28 H 0.144293	28 H 0.162907
29 H 0.052332	29 H 0.035003	29 H -0.004705	29 H 0.075910	29 H 0.058354	29 H 0.017199
30 C -0.179237	30 C -0.177339	30 C -0.173132	30 C -0.211776	30 C -0.210418	30 C -0.205017
31 H 0.142457	31 H 0.147342	31 H 0.163199	31 H 0.154928	31 H 0.165940	31 H 0.178965
32 H 0.116911	32 H 0.125758	32 H 0.148061	32 H 0.141929	32 H 0.154125	32 H 0.174254
33 C -0.053794	33 C -0.053111	33 C -0.051814	33 C -0.093587	33 C -0.093933	33 C -0.092597
34 H 0.044827	34 H 0.031738	34 H -0.001054	34 H 0.065708	34 H 0.048925	34 H 0.017745
35 H 0.033367	35 H 0.012592	35 H -0.037668	35 H 0.049446	35 H 0.025893	35 H -0.023427
36 H 0.104548	36 H 0.111710	36 H 0.128182	36 H 0.130263	36 H 0.138965	36 H 0.154263
37 H 0.044903	37 H 0.031984	37 H 0.000021	37 H 0.060893	37 H 0.045423	37 H 0.014350
38 H 0.108197	38 H 0.113133	38 H 0.128356	38 H 0.128960	38 H 0.138533	38 H 0.150504
39 C -0.163031	39 C -0.153324	39 C -0.134679	39 C -0.195782	39 C -0.188200	39 C -0.166582
40 H 0.098906	40 H 0.101269	40 H 0.107402	40 H 0.119721	40 H 0.124572	40 H 0.128930
41 H 0.047198	41 H 0.033996	41 H 0.002375	41 H 0.061222	41 H 0.045342	41 H 0.015946
42 C -0.173259	42 C -0.168094	42 C -0.152930	42 C -0.212293	42 C -0.206719	42 C -0.188584
43 H 0.060239	43 H 0.033039	43 H -0.026513	43 H 0.076350	43 H 0.051230	43 H -0.010903
44 H 0.120636	44 H 0.110699	44 H 0.095774	44 H 0.144918	44 H 0.143625	44 H 0.120589
45 C -0.164329	45 C -0.130985	45 C -0.063677	45 C -0.204736	45 C -0.179411	45 C -0.119806
46 H 0.053626	46 H -0.000115	46 H -0.107504	46 H 0.074823	46 H 0.031747	46 H -0.068210
47 H 0.109837	47 H 0.090357	47 H 0.063287	47 H 0.129836	47 H 0.119381	47 H 0.088660
48 C -0.153770	48 C -0.084672	48 C 0.029987	48 C -0.201447	48 C -0.141353	48 C -0.002944
49 H 0.112079	49 H 0.047001	49 H -0.063002	49 H 0.131817	49 H 0.084663	49 H -0.044675
50 H 0.052262	50 H -0.082993	50 H -0.387744	50 H 0.072006	50 H -0.033825	50 H -0.370746
51 C -0.305823	51 C -0.064645	51 C 0.391404	51 C -0.350730	51 C -0.165054	51 C 0.356742
52 H 0.062372	52 H -0.179984	52 H -0.652280	52 H 0.078668	52 H -0.109043	52 H -0.654441
53 H 0.118301	53 H -0.020211	53 H -0.274262	53 H 0.136540	53 H 0.033616	53 H -0.270691
54 C 0.095743	54 C 0.214088	54 C 0.467443	54 C 0.107604	54 C 0.190628	54 C 0.467724
55 N -0.229026	55 N -0.103663	55 N 0.174442	55 N -0.232276	55 N -0.121292	55 N 0.193592
56 H 0.130823	56 H 0.151971	56 H 0.195062	56 H 0.158605	56 H 0.177896	56 H 0.222579
57 H 0.065007	57 H 0.061241	57 H 0.048161	57 H 0.082942	57 H 0.074585	57 H 0.063467
58 H 0.110059	58 H 0.120694	58 H 0.144715	58 H 0.129450	58 H 0.141187	58 H 0.165084
59 H 0.049405	59 H 0.039997	59 H 0.014747	59 H 0.071997	59 H 0.058584	59 H 0.034765
60 H 0.031823	60 H -0.279986	60 H -0.903315	60 H 0.051723	60 H -0.198718	60 H -0.886788

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