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The First Synthesis of Some Novel 4-Chloro Chalcone Based Oxime Ethers: An Experimental and Computational Study

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Oxime ether,
DFT calculation,
Computational chemistry

Abstract: In this study; a series of novel oxime ethers, 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one *O*-benzyl oximes, have been synthesized and characterized by several spectroscopic methods. To the best of our knowledge, this is the first synthesis of 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one *O*-benzyl oximes. The study consists of two parts. In the first part, the synthesis and the characterization of the selected compounds have been carried out. In the second part of our study some DFT (Density Functional Theory) calculations have been performed on the synthesized molecules and the obtained results have been compared with the experimental results. In the study; single point energy calculations, geometry optimizations, frequency analysis, NMR spectral analysis, molecular electrostatic potential map calculations, frontier molecular orbital calculations, determination of some global reactivity descriptors and Mulliken atomic charge calculations have been performed. All DFT calculations were carried out at the B3LYP/6-31G(d), B3LYP/6-311G(d,p) and B3LYP/6-311+G(2d,p) level of theories.

Bazı Yeni 4-Klor Kalkon Bazlı Oksim Eterlerin İlk Sentezi: Bir Deneysel ve Hesapsal Çalışma

Anahtar Kelimeler
Kalkon,
Oksim,
Oksim eter,
DFT hesaplama,
Hesapsal kimya

Özet: Bu çalışmada; bir seri yeni oksim eterler, 3-(4-klorfenil)-1-fenil-2-propen-1-on *O*-benzil oksimler, sentezlenmiş ve çeşitli spektroskopik yöntemlerle karakterize edilmiştir. Bildiğimiz kadarıyla bu, 3-(4-klorfenil)-1-fenilprop-2-en-1-on *O*-benzil oksimlerin ilk sentezidir. Bu çalışma iki kısımdan oluşmaktadır. Birinci kısımda seçilen bileşiklerin sentezleri ve karakterizasyonları gerçekleştirilmiştir. Çalışmamızın ikinci kısmında ise sentezlenen moleküller üzerinde bazı DFT (Yoğunluk Fonksiyonel Teorisi) hesaplamaları gerçekleştirilmiş ve elde edilen sonuçlar deneysel sonuçlarla karşılaştırılmıştır. Çalışmada; tek nokta enerji hesaplamaları, geometri optimizasyonları, frekans analizleri, NMR spektral analizleri, moleküler elektrostatik potansiyel haritası hesaplamaları, sınır moleküler orbital hesaplamaları, bazı global reaktivite tanımlayıcıların belirlenmesi ve Mulliken atomik yük hesaplamaları gerçekleştirilmiştir. Tüm DFT hesaplamaları B3LYP/6-31G(d), B3LYP/6-311G(d,p) ve B3LYP/6-311+G(2d,p) teori düzeylerinde gerçekleştirilmiştir.

1. Introduction

Chalcones are important compounds in organic synthesis because of being important precursors of some important organic compounds such as flavonoids and isoflavonoids. Chalcones can be found widespread in natural products [1] and they have broad spectrum of biological activity [2, 3] Recent studies showed that chalcones are promising anticancer [4], antimalarial [5-7], antiinflammatory [8], antitubercular [9], antihyperglycemic [10] and antimitotic agents. [11]

Oximes and related compounds are of significant interest because of their synthetic values as intermediates in organic synthesis and their industrial importance. [12] Chalcone oximes are also important compounds in organic chemistry. [13, 14].

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In this study, some novel 4-chloro chalcone based oxime ethers, **6a-e**, were synthesized and characterized. To the best of our knowledge this is the first synthesis of 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one *O*-benzyl oximes, **6a-e**. In Figure 1, a typical chalcone structure and its oxime and oxime ether forms are represented.

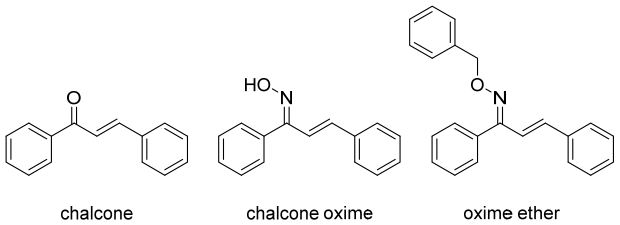
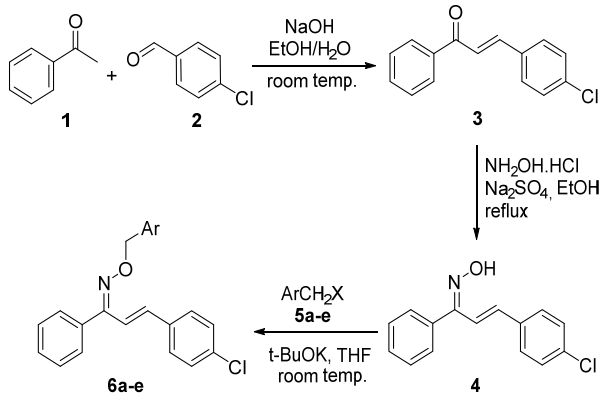


Figure 1. A typical chalcone and its oxime and oxime ether forms.

2. Material and Method

2.1. Experimental

The literature contains several reports on the synthesis of chalcones from corresponding ketones and aldehydes [2, 15-17] and on the synthesis of chalcone oximes from corresponding chalcones [18-21]. The synthetic pathway for the synthesis of novel 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one *O*-benzyl oximes was given in Figure 2.



Comp.	Ar
6a	-phenyl
6b	-4-chlorophenyl
6c	-2,4-dichlorophenyl
6d	-3,4-dichlorophenyl
6e	-2,6-dichlorophenyl

Comp.	Ar	X
5a	-phenyl	Br
5b	-4-chlorophenyl	Cl
5c	-2,4-dichlorophenyl	Cl
5d	-3,4-dichlorophenyl	Cl
5e	-2,6-dichlorophenyl	Cl

Figure 2. Synthetic pathway.

In the synthesis of chalcone **3** from corresponding ketone **1** and aldehyde **2**, a well known condensation method, Claisen-Schmidt condensation, was used. In the synthesis of oxime **4**, from corresponding ketone **3**, hydroxylaminehydrogenchloride and sodium sulfate was used and the reaction carried out at reflux temperature in ethanol. [12] In the synthesis of oxime ethers **6a-e** from corresponding oxime **4** and aryl halide **5a-e**, t-BuOK was used as a base and the reaction was carried out in THF at room temperature.

*Procedure for the synthesis of (E)-3-(4-chlorophenyl)-1-phenyl-2-propen-1-one, **3***

To a solution of acetophenone (10 mmol) in ethanol (15 mL) and water (15 mL) NaOH (15 mmol) was added portionwise at room temperature with continuous stirring. After 5 minutes, 4-chlorobenzaldehyde (10 mmol) was added portionwise in 5 minutes time. After completion of the reaction, the formed solids were filtrated and recrystallized from ethanol.

*Synthesis of 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one oxime, **4***

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one (4 mmol), hydroxylamine hydrochloride (6 mmol) and sodium sulfate (4 mmol) dissolved in ethanol (25 mL) and refluxed for 5 hours. The reaction mixture was filtrated and the solvent was evaporated under reduced pressure at the end of reflux time. Then water was added, extracted with dichloromethane, dried over anhydrous sodium sulfate and evaporation of the solvent under reduced pressure gave crude product. The crude product was purified by column chromatography on silica gel, eluted with a mixture of Hex:EtOAc (10:1). 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one oxime was obtained as a mixture of (*E*)- and (*Z*)- isomers (The molar ratio of *E/Z* isomers is 70:30).

*Synthesis of 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-benzyl oximes, **6a-e***

To a solution of 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one oxime, **4** (2 mmol) in THF (20 mL), t-BuOK (2 mmol) was added portionwise with continuous stirring. After 10 minutes, corresponding benzyl halide **5a-e** (2 mmol) was added portionwise. After 2 hours of stirring at room temperature 5 mL of methanol was added and the solvent was evaporated under reduced pressure. Then water was added, extracted with dichloromethane, dried over anhydrous sodium sulfate and evaporation of the solvent under reduced pressure gave crude product. The product was purified by column chromatography with a mixture of Hex:EtOAc (10:1).

2.2. Theoretical calculations

In the second part of our study we have done some density functional theory (DFT) calculations on the selected molecules **3**, **4** and **6a-e** and we have made a comparison between experimental and theoretical data. Geometry optimization and frequency analysis were carried out at the DFT B3LYP/6-31G(d), B3LYP/6-311G(d,p) and B3LYP/6-311+G(2d,p) level of theories. NMR calculations were also performed at the same level of theories using both GIAO (Gauge-Independent Atomic Orbital) and CSGT (Continuous Set of Gauge Transformations) models. All theoretical calculations have been performed using Gaussian 09,

Revision D.01 Program Package [22] and GaussView5 [23] was used for the visualization of the computational results.

3. Results

3.1. Experimental results

(E)-3-(4-chlorophenyl)-1-phenyl-2-propen-1-one, ***3***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 8.03 (dd, J=8 and 1.4 Hz, 2H), 7.78 (d, J=16 Hz, 1H), 7.64-7.50 (m, 6H), 7.40 (d, J=8 Hz, 2H); m/z (ESI): 243 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one oxime, ***4***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 9.30 (br, 2.4H), 7.68 (d, J=16.4Hz, 2.4H), 7.56-7.25 (m, 30.6H), 7.07 (d, J=16.4 Hz, 1H), 6.78 (d, 16.4 Hz, 2.4H), 6.46 (d, 16.4 Hz, 1H); m/z (ESI): 258 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-benzyl oxime, ***6a***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.63 (d, 3.4H, J=16.6 Hz), 7.55-7.25 (m, 62H), 7.05 (d, 1H, J=16.6 Hz), 6.74 (d, 3.4H, J=16.4 Hz), 6.40 (d, 1H, J=16.4 Hz), 5.34 (s, 6.8H), 5.20 (s, 2H); m/z (ESI): 348 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-(4-chlorobenzyl) oxime, ***6b***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.80-7.15 (m, 55H), 7.02 (d, 1H, J=16.4 Hz), 6.72 (d, 3H, J=16.4 Hz), 6.38 (d, 1H, J=16.4 Hz), 5.26 (s, 6H), 5.13 (s, 2H); m/z (ESI): 382 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-(2,4-dichlorobenzyl) oxime, ***6c***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.67-7.17 (m, 51H), 7.05 (d, 1H, J=16.4 Hz), 6.74 (d, 3H, J=16.4 Hz), 6.40 (d, 1H, J=16.4 Hz), 5.41 (s, 6H), 5.27 (s, 2H); m/z (ESI): 416 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-(3,4-dichlorobenzyl) oxime, ***6d***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.65-7.10 (m, 51H), 7.04 (d, 1H, J=16.4 Hz), 6.73 (d, 3H, J=16.4 Hz), 6.40 (d, 1H, J=16.4 Hz), 5.23 (s, 6H), 5.09 (s, 2H); m/z (ESI): 416 $[M-H]^+$.

3-(4-chlorophenyl)-1-phenyl-2-propen-1-one O-(2,6-dichlorobenzyl) oxime, ***6e***

^{1}H-NMR ($CDCl_3$, 300 MHz) δ, 7.65-7.14 (m, 43.2H), 7.02 (d, 1H, J=16.4 Hz), 6.72 (d, 2.4H, J=16.4 Hz), 6.40 (d, 1H, J=16.4 Hz), 5.58 (s, 4.8H), 5.43 (s, 2H); m/z (ESI): 416 $[M-H]^+$.

3.2. Computational results

Single Point Energies for Optimized Structures

Single point energies of the compounds 3, 4 and 6a-e were calculated at the DFT B3LYP/6-31G(d), B3LYP/6-311G(d,p) and B3LYP/6-311+G(2d,p) level of theories and single point energies for compounds 3 and 4 were given in Table 1.

Table 1. Calculated energies for the (*E*)- and (*Z*)-isomers of compound 3 and 4.

Comp.	6-31G(d)	6-311G(d,p)	6-311+G(2d,p)
(E)-3	-30068.109103	-30073.171799	-30073.949982
(Z)-3	-30067.923036	-30072.985377	-30073.745275
ΔE	0.186067	0.186422	0.204707
(E)-4	-31561.029634	-31566.614994	-31567.520975
(Z)-4	-31560.990671	-31566.583433	-31567.502759
ΔE	0.038962	0.031561	0.018216

Optimized Structure Analysis

Geometric parameters such as bond lengths, bond angles and dihedral angles were determined theoretically at the same level of theories. The calculated molecular structures and molecular parameters of compounds 3, (*E*)-4, (*Z*)-4, (*E*)-6a and (*Z*)-6a at the B3LYP/6-311+G(2d,p) level of theory were given in Appendices.

Frequency Analysis

Frequency analysis for the compounds 3, 4 and 6a-e were carried out at the same level of theories. As an example calculated IR spectra for compound 6a was given in Figure 3.

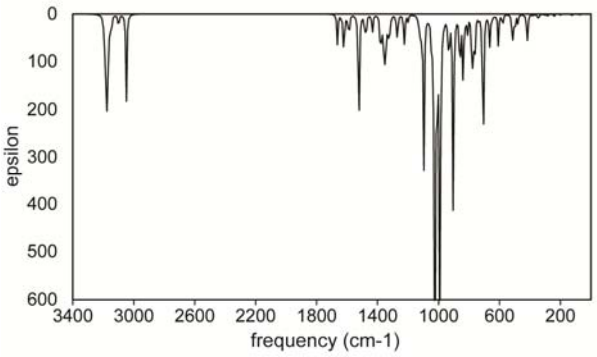


Figure 3. Calculated IR spectra for the compound 6a.

NMR Spectral Analysis

Nuclear magnetic shield tensors were computationally determined at the same level of theories using both GIAO (Gauge-Independent Atomic Orbital) and CSGT (Continuous Set of Gauge Transformations) models. Calculated and experimental ^{1}H-NMR chemical shifts for compounds (*E*)-6a and (*Z*)-6a were given in Table 2 and Table 3, respectively.

Table 2. Experimental and Calculated ^{1}H-NMR Chemical Shifts for Compound (*E*)-6a.

Atom	Exp.	G1	G2	G3	C1	C2	C3
26-H	7.63	7.36	7.85	8.00	4.27	6.24	7.54
27-H	7.55-7.25	7.44	7.69	7.75	4.73	6.42	7.40
28-H	7.55-7.25	7.25	7.55	7.64	4.69	6.34	7.30
29-H	7.55-7.25	7.27	7.57	7.67	4.71	6.34	7.33
30-H	7.55-7.25	7.25	7.55	7.64	4.69	6.34	7.30
31-H	7.55-7.25	7.44	7.69	7.75	4.73	6.42	7.40
32-H	6.74	6.29	6.62	6.78	3.54	5.33	6.41
33-H	7.55-7.25	7.12	7.44	7.61	4.24	5.96	7.20
34-H	7.55-7.25	6.99	7.31	7.51	3.79	5.64	7.00
35-H	7.55-7.25	6.99	7.31	7.51	3.79	5.64	7.00
36-H	7.55-7.25	7.12	7.44	7.61	4.24	5.96	7.20
37-H	5.34	5.12	5.27	5.33	3.09	4.13	5.06
38-H	5.34	5.12	5.27	5.33	3.09	4.13	5.06
39-H	7.55-7.25	7.35	7.66	7.75	4.74	6.42	7.43
40-H	7.55-7.25	7.17	7.46	7.56	4.66	6.28	7.22
41-H	7.55-7.25	7.17	7.46	7.57	4.66	6.28	7.23
42-H	7.55-7.25	7.17	7.46	7.56	4.66	6.28	7.22
43-H	7.55-7.25	7.35	7.66	7.75	4.74	6.42	7.43

Exp.: Experimental
G1: GIAO 6-31G(d)
G2: GIAO 6-311G(d,p)
G3: GIAO 6-311+G(2d,p)
C1: CSGT 6-31G(d)
C2: CSGT 6-311G(d,p)
C3: CSGT 6-311+G(2d,p)

Table 3. Experimental and Calculated ^{1}H-NMR Chemical Shifts for Compound (*Z*)-6a.

Atom	Exp.	G1	G2	G3	C1	C2	C3
26-H	7.55-7.25	7.14	7.44	7.56	4.63	6.26	7.19
27-H	7.55-7.25	7.14	7.43	7.52	4.63	6.23	7.20
28-H	7.55-7.25	7.14	7.44	7.56	4.63	6.26	7.19
29-H	7.55-7.25	7.32	7.57	7.68	4.69	6.39	7.26
30-H	7.55-7.25	7.32	7.57	7.68	4.69	6.39	7.26
31-H	6.40	6.36	6.69	6.82	3.36	5.28	6.44
32-H	7.05	7.16	7.58	7.65	4.13	5.96	7.33
33-H	5.20	4.97	5.11	5.13	2.94	3.97	4.90
34-H	5.20	4.97	5.11	5.13	2.94	3.97	4.90
35-H	7.55-7.25	7.20	7.53	7.72	4.27	6.02	7.30
36-H	7.55-7.25	7.02	7.36	7.51	3.80	5.65	7.05
37-H	7.55-7.25	7.02	7.36	7.51	3.80	5.65	7.05
38-H	7.55-7.25	7.20	7.53	7.72	4.27	6.02	7.30
39-H	7.55-7.25	7.47	7.79	7.86	4.85	6.54	7.54
40-H	7.55-7.25	7.27	7.56	7.64	4.74	6.37	7.32
41-H	7.55-7.25	7.23	7.54	7.66	4.72	6.34	7.31
42-H	7.55-7.25	7.27	7.56	7.64	4.74	6.37	7.32
43-H	7.55-7.25	7.47	7.79	7.86	4.85	6.54	7.54

Exp.: Experimental
G1: GIAO 6-31G(d)
G2: GIAO 6-311G(d,p)
G3: GIAO 6-311+G(2d,p)
C1: CSGT 6-31G(d)
C2: CSGT 6-311G(d,p)
C3: CSGT 6-311+G(2d,p)

Molecular Electrostratic Potential Maps

Molecular electrostatic potential maps provides information about the electron rich and electron deficient parts of the investigated molecule. Molecular electrostatic potential maps were calculated at the same leve of theories. Calculated MEP diagrams for compound 3, (*E*)-4, (*Z*)-4, (*E*)-6a and (*Z*)-6a at the B3LYP/6-311+G(2d,p) level of theory were given in Figure 4, 5, 6, 7 and 8, respectively.

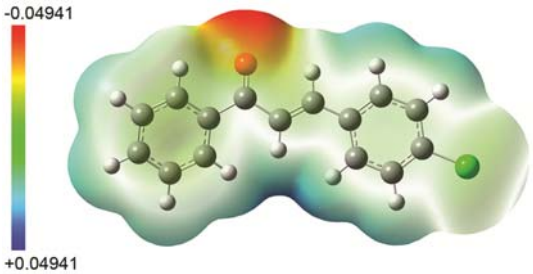


Figure 4. Calculated MEP map for compound 3.

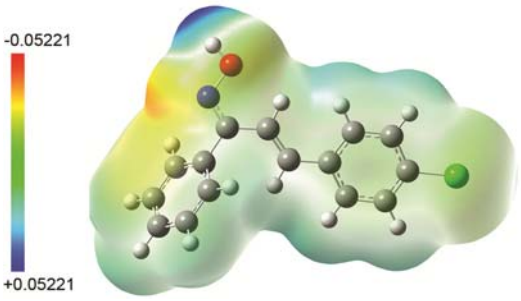


Figure 5. Calculated MEP map for compound (*E*)-4.

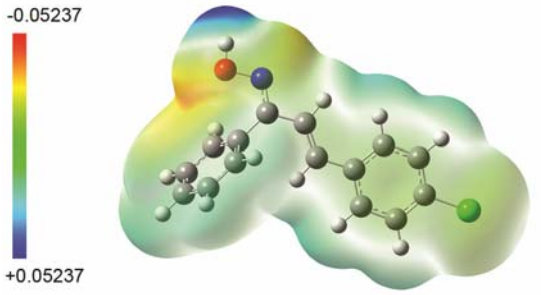


Figure 6. Calculated MEP map for compound (*Z*)-4.

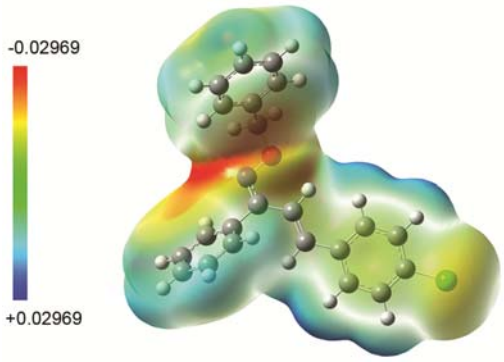


Figure 7. Calculated MEP map for compound (*E*)-6a.

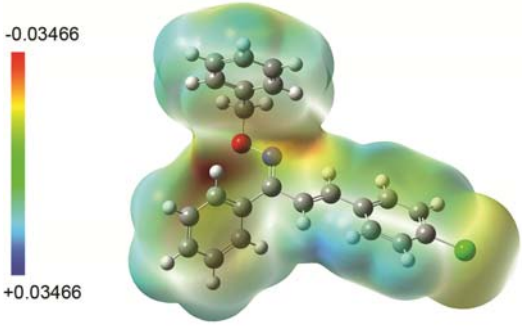


Figure 8. Calculated MEP map for compound (*Z*)-6a.

Frontier molecular orbitals and global reactivity descriptors

LUMO and HOMO calculations were carried out at the same level of theories. HOMO and LUMOs of compound 3, (*E*)-4, (*Z*)-4, (*E*)-6a and (*Z*)-6a at the B3LYP/6-311+G(2d,p) level of theory were given in Figure 9, 10, 11, 12 and 13, respectively.

Ionization potential (I), electron affinity (A), electronegativity (χ), chemical hardness (η), chemical softness (S), electronic potential (μ) and electrophilicity index (ω) values were determined and given for the compounds 3, (*E*)-4, (*Z*)-4, (*E*)-6a and (*Z*)-6a in Table 4.

Ionization potential is the minimum energy required to remove an electron from an atom or molecule and can be calculated with Eq. (1) and electron affinity is the amount of energy released when an electron is added to a neutral atom or molecule in the gaseous state and can be calculated with Eq. (2). [24]

$$I = -E_{HOMO} \quad (1)$$

$$A = -E_{LUMO} \quad (2)$$

Electronegativity, chemical hardness, chemical softness, electronic chemical potential and electrophilic index can be calculated with Eq.(3)-Eq.(7). [24-31]

$$\chi = (I + A)/2 \quad (3)$$

$$\eta = (I - A)/2 \quad (4)$$

$$S = 1/2\eta \quad (5)$$

$$\mu = -(I + A)/2 \quad (6)$$

$$\omega = \mu^2/2\eta \quad (7)$$

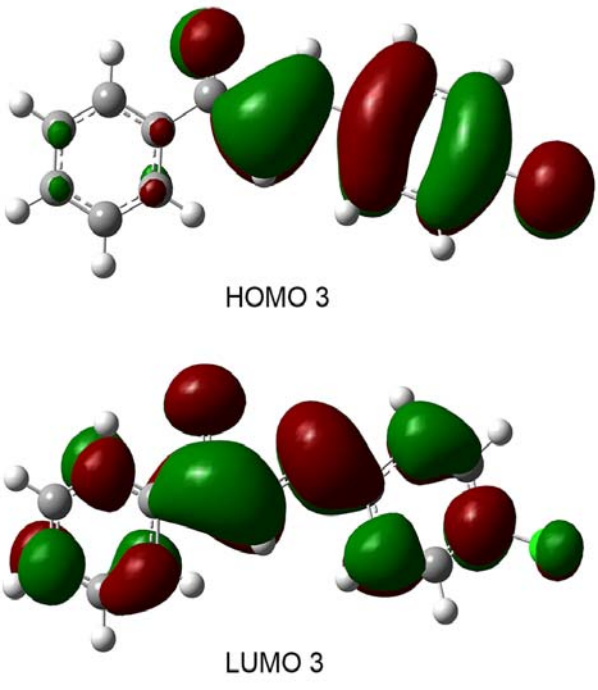


Figure 9. Calculated HOMO and LUMOs of Compound 3.

Mulliken Atomic Charges

The Mulliken charge distribution of the synthesized molecules were determined theoretically at the same level of theories. The Mulliken atomic charges for compounds (*E*)-6a and (*Z*)-6a were given in Figure 14 and Figure 15, respectively.

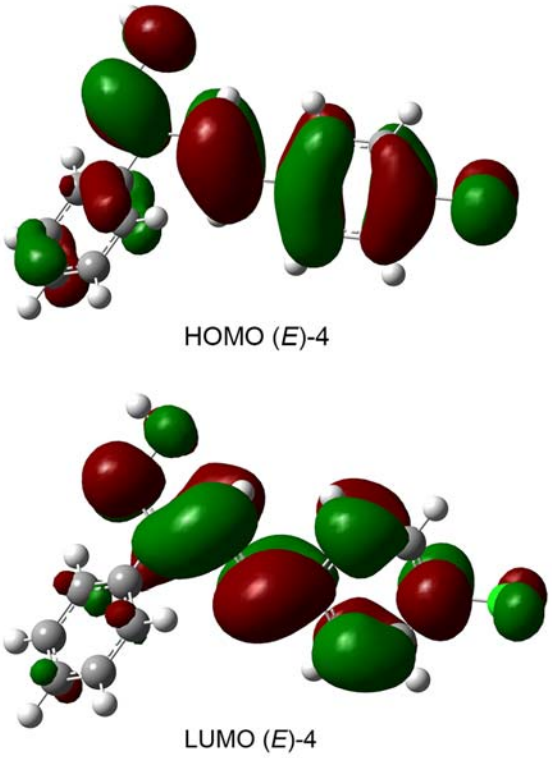


Figure 10. Calculated HOMO and LUMOs of Compound (*E*)-4.

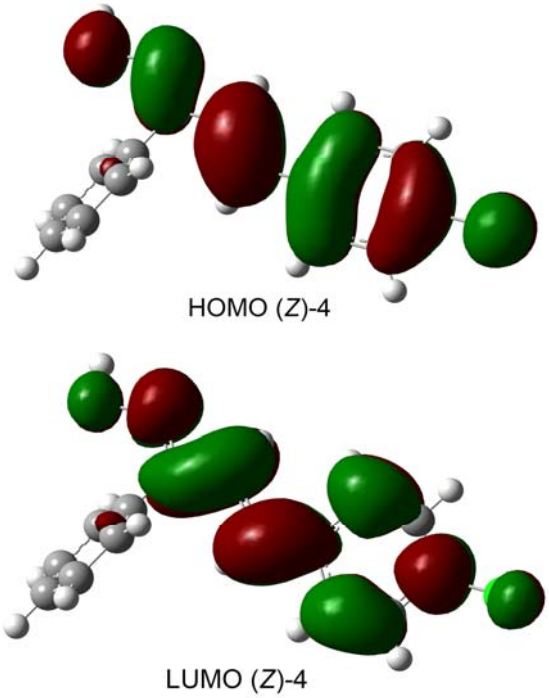


Figure 11. Calculated HOMO and LUMOs of Compound (*Z*)-4.

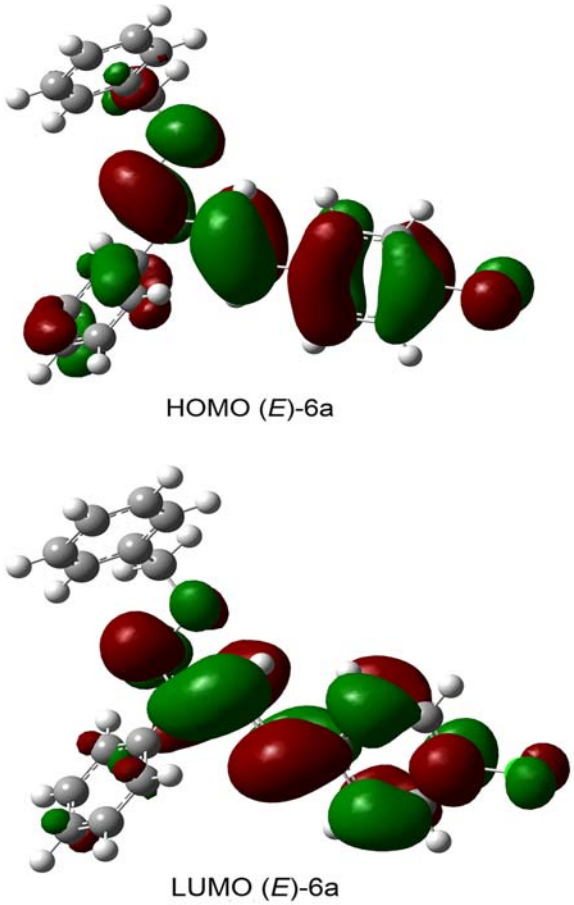


Figure 12. Calculated HOMO and LUMOs of Compound (*E*)-6a.

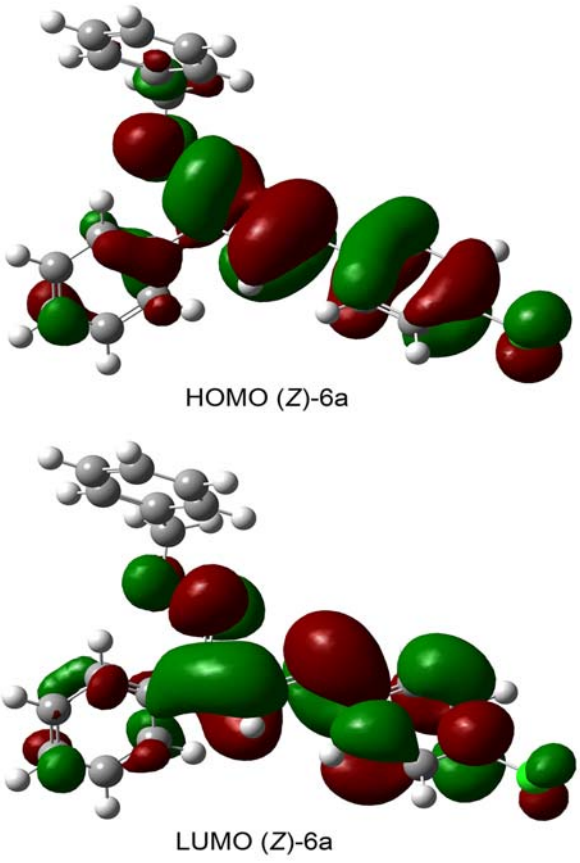


Figure 13. Calculated HOMO and LUMOs of Compound (*Z*)-6a.

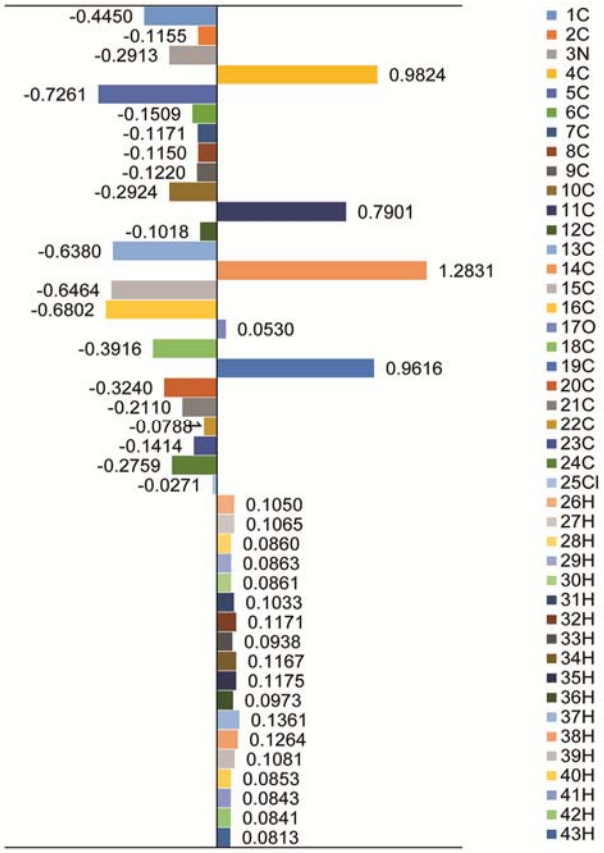


Figure 14. Calculated HOMO and LUMOs of Compound (*E*)-6a.

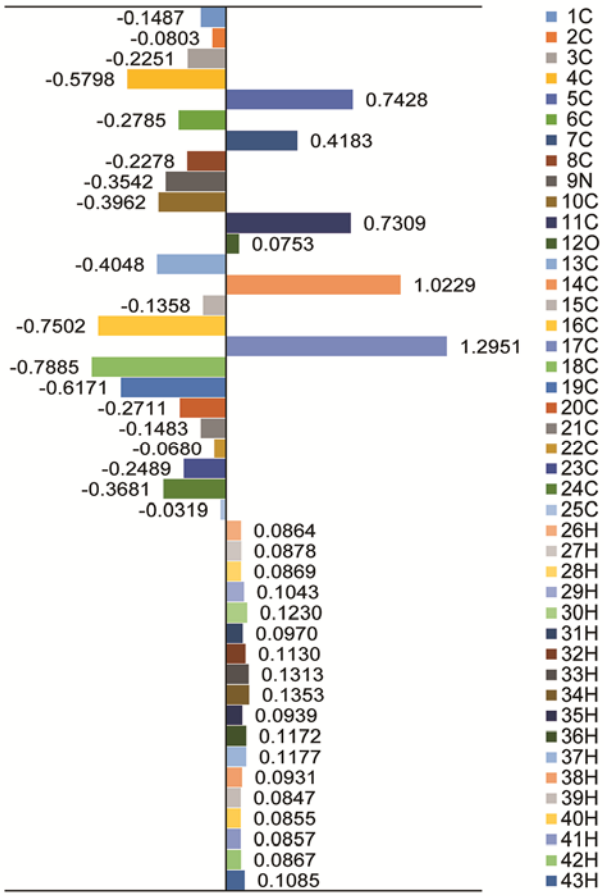


Figure 15. Calculated HOMO and LUMOs of Compound (*Z*)-6a.

Table 4. Global Reactivity Descriptors (6-311+G(2d,p))

	Comp.3	Comp. (*E*)-4	Comp. (*Z*)-4	Comp. (*E*)-6a	Comp. (*Z*)-6a
LUMO	2.63304	-2.15352	-1.98774	-2.10546	-2.03607
HOMO	-6.642	-6.17112	-6.07527	-6.03396	-5.96592
HOMO-LUMO Gap	9.27504	4.0176	4.08753	3.9285	3.92985
I	6.642	6.17112	6.07527	6.03396	5.96592
A	-2.63304	2.15352	1.98774	2.10546	2.03607
χ	2.00448	4.16232	4.031505	4.06971	4.000995
η	4.63752	2.0088	2.043765	1.96425	1.964925
S	0.107816247	0.248904819	0.244646522	0.254550083	0.254462639
μ	-2.00448	-4.16232	-4.031505	-4.06971	-4.000995
ω	0.433199218	4.312253032	3.976247897	4.215995796	4.073427991

4. Discussion and Conclusion

In conclusion, we have prepared some novel chalcone based oxime ethers, 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one *O*-benzyl oximes and we have characterized them using various characterization methods. We have also carried out some DFT calculations on the synthesized molecules.

In the synthesis of chalcone **3** from corresponding ketone **1** and aldehyde **2**, the only product is (*E*)-isomer. It is not surprising to obtain only (*E*)-isomer because of its more stable molecular structure than the (*Z*)-isomer. The DFT calculations also support these experimental results. In all cases, the (*E*)-isomers were approximately 0.2 eV lower in energy from the (*Z*)-isomers. The energies calculated for the (*E*)- and (*Z*)-isomers of the compound **3** at the B3LYP/6-31G(d), B3LYP/6-311G(d,p) and B3LYP/6-311+G(2d,p) level of theories and the energy difference between (*E*)- and (*Z*)-isomers were given in Table 1.

In the synthesis of compound **4** from corresponding chalcone **3**, the product is a mixture of (*E*)- and (*Z*)-isomers. The *E:Z* molar ratio was found to be approximately 70:30. In all cases, the calculated energies for (*E*)-isomers were lower than the energies for (*Z*)-isomers but this energy differences are relatively small compared to the energy differences between the (*E*)- and (*Z*)-isomers of chalcone **3**. This explains why (*E*)-isomer is not the only product in the conversion of chalcone to the corresponding chalcone oxime. The energies calculated for the (*E*)- and (*Z*)-isomers of the compound **4** and the energy difference between (*E*)- and (*Z*)-isomers were given in Table 1.

In the NMR spectral analysis, it can be said that there was a good agreement between the computational and experimental results. For the CSGT based NMR calculations it was found that the higher basis sets gave the best results. In GIAO based NMR calculations especially for certain protons the higher basis set overestimate the chemical shifts. When compared to the experimental values, it can be said that the best computational methods for the estimation of chemical shifts for the synthesized molecules are DFT B3LYP/6-311G(d,p) GIAO and DFT B3LYP/6-311+G(2d,p) CSGT.

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Appendices

Appendix A. Calculated Molecular Structures

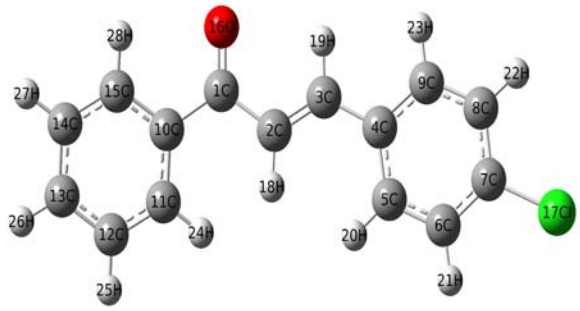

Figure A.1. Calculated Molecular Structure of Compound 3.

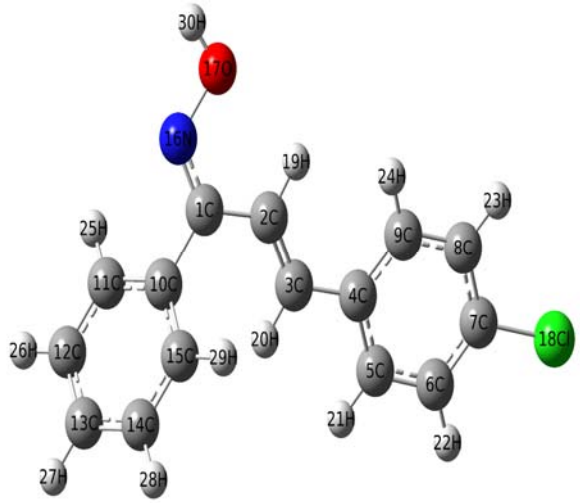

Figure A.2. Calculated Molecular Structure of Compound (*E*)-4.

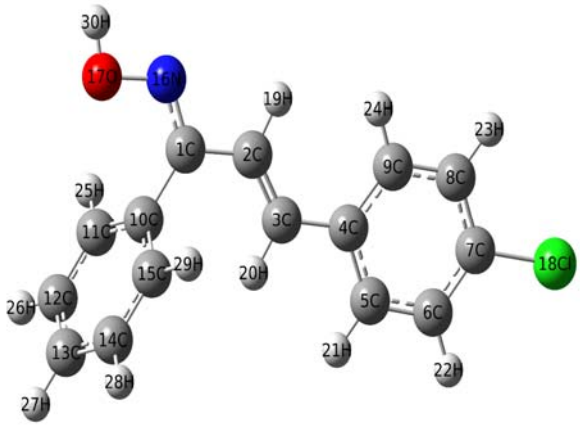

Figure A.3. Calculated Molecular Structure of Compound (*Z*)-4.

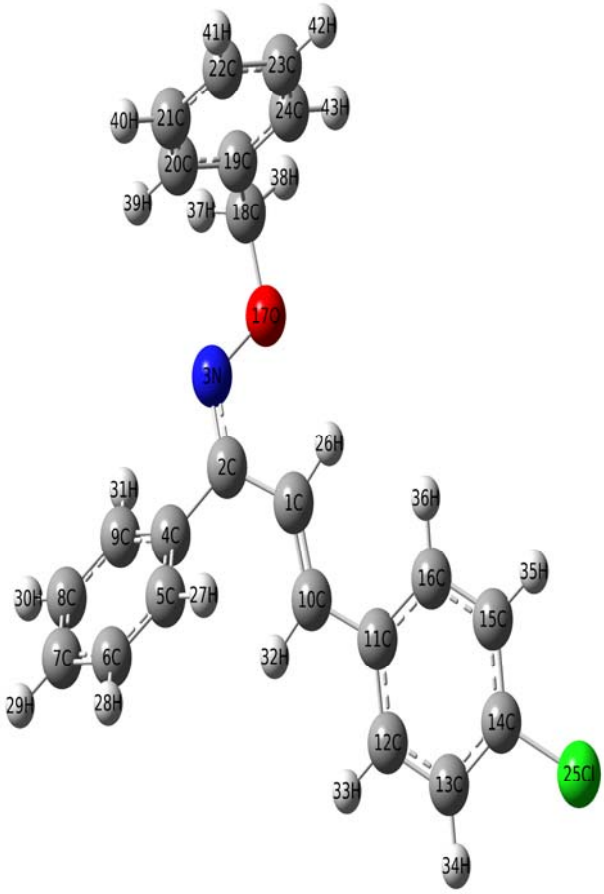

Figure A.4. Calculated Molecular Structure of Compound (*E*)-6a.

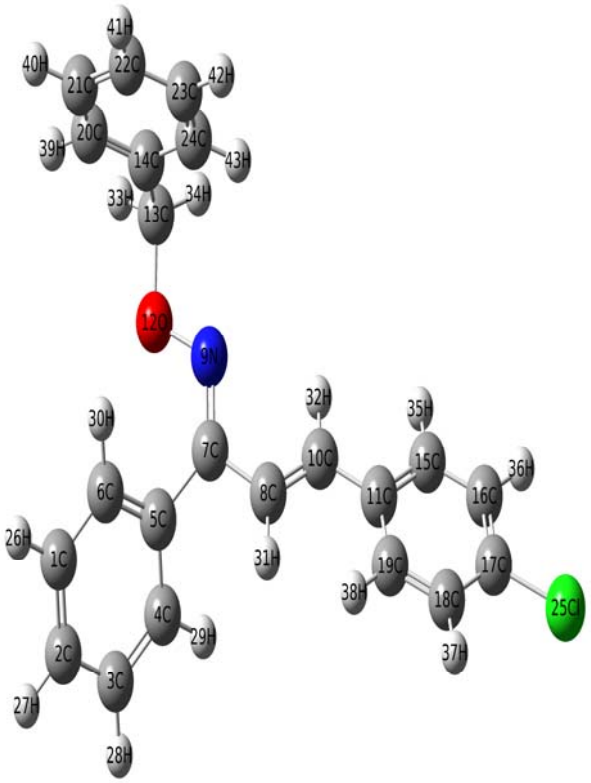

Figure A.5. Calculated Molecular Structure of Compound (*Z*)-6a.

Appendix B. Calculated Geometric Parameters

Table B.1. Calculated Bond Lengths, Bond Angels and Dihedral Angles for Compound 3.

Atoms	Bond Length	Atoms	Bond Angle	Atoms	Dihedral Angle
C15-H28	1.082	H28-C15-C14	121.13	C13-C14-C15-C10	-0.61
C14-H27	1.083	H28-C15-C10	118.21	C13-C14-C15-H28	179.34
C14-C15	1.386	C14-C15-C10	120.66	H27-C14-C15-C10	179.52
C13-H26	1.084	H27-C14-C15	119.92	H27-C14-C15-H28	-0.53
C13-C14	1.394	H27-C14-C13	120.02	C12-C13-C14-C15	0.05
C12-H25	1.083	C15-C14-C13	120.07	C12-C13-C14-H27	179.92
C12-C13	1.390	H26-C13-C14	120.11	H26-C13-C14-C15	-179.82
C11-H24	1.082	H26-C13-C12	120.04	H26-C13-C14-H27	0.05
C11-C12	1.391	C14-C13-C12	119.85	C11-C12-C13-C14	0.52
C10-C15	1.400	H25-C12-C13	120.12	C11-C12-C13-H26	-179.61
C10-C11	1.399	H25-C12-C11	119.81	H25-C12-C13-C14	-179.42
C9-H23	1.084	C13-C12-C11	120.08	H25-C12-C13-H26	0.45
C8-H22	1.082	H24-C11-C12	118.77	C10-C11-C12-C13	-0.54
C8-C9	1.388	H24-C11-C10	120.67	C10-C11-C12-H25	179.40
C7-Cl17	1.753	C12-C11-C10	120.54	H24-C11-C12-C13	-179.26
C7-C8	1.387	C15-C10-C11	118.79	H24-C11-C12-H25	0.68
C6-H21	1.082	C15-C10-C1	117.72	C1-C10-C15-C14	179.55
C6-C7	1.392	C11-C10-C1	123.48	C1-C10-C15-H28	-0.40
C5-H20	1.083	H23-C9-C8	119.20	C11-C10-C15-C14	0.59
C5-C6	1.384	H23-C9-C4	119.18	C11-C10-C15-H28	-179.37
C4-C9	1.402	C8-C9-C4	121.62	C1-C10-C11-C12	-178.91
C4-C5	1.404	H22-C8-C9	120.80	C1-C10-C11-H24	-0.22
C3-H19	1.087	H22-C8-C7	120.20	C15-C10-C11-C12	-0.01
C3-C4	1.459	C9-C8-C7	119.00	C15-C10-C11-H24	178.68
C2-H18	1.081	Cl17-C7-C8	119.64	C7-C8-C9-C4	-0.02
C2-C3	1.342	Cl17-C7-C6	119.40	C7-C8-C9-H23	-180.00
C1-O16	1.223	C8-C7-C6	120.96	H22-C8-C9-C4	179.98
C1-C10	1.501	H21-C6-C7	119.93	H22-C8-C9-H23	0.01
C1-C2	1.484	H21-C6-C5	120.70	C6-C7-C8-C9	-0.04
		C7-C6-C5	119.37	C6-C7-C8-H22	179.96
		H20-C5-C6	118.61	Cl17-C7-C8-C9	179.99
		H20-C5-C4	120.13	Cl17-C7-C8-H22	-0.02
		C6-C5-C4	121.27	C5-C6-C7-C8	0.04
		C9-C4-C5	117.78	C5-C6-C7-Cl17	-179.98
		C9-C4-C3	118.67	H21-C6-C7-C8	-179.91
		C5-C4-C3	123.55	H21-C6-C7-Cl17	0.07
		H19-C3-C4	115.92	C4-C5-C6-C7	0.02
		H19-C3-C2	116.13	C4-C5-C6-H21	179.97
		C4-C3-C2	127.95	H20-C5-C6-C7	-179.92
		H18-C2-C3	121.05	H20-C5-C6-H21	0.03
		H18-C2-C1	118.64	C3-C4-C9-C8	-179.90
		C3-C2-C1	120.30	C3-C4-C9-H23	0.07
		O16-C1-C10	119.88	C5-C4-C9-C8	0.08
		O16-C1-C2	121.12	C5-C4-C9-H23	-179.94
		C10-C1-C2	119.00	C3-C4-C5-C6	179.90
				C3-C4-C5-H20	-0.16
				C9-C4-C5-C6	-0.08
				C9-C4-C5-H20	179.86
				C2-C3-C4-C5	-0.44
				C2-C3-C4-C9	179.54
				H19-C3-C4-C5	179.46
				H19-C3-C4-C9	-0.55
				C1-C2-C3-C4	179.12
				C1-C2-C3-H19	-0.78
				H18-C2-C3-C4	0.38
				H18-C2-C3-H19	-179.53
				C2-C1-C10-C11	-14.79
				C2-C1-C10-C15	166.30
				O16-C1-C10-C11	166.05
				O16-C1-C10-C15	-12.86
				C10-C1-C2-C3	177.31
				C10-C1-C2-H18	-3.92
				O16-C1-C2-C3	-3.55
				O16-C1-C2-H18	175.23

Table B.2. Calculated Bond Lengths, Bond Angels and Dihedral Angles for Compound (*E*)-4

Atoms	Bond Length	Atoms	Bond Angle	Atoms	Dihedral Angle
O17-H30	0.964	H30-O17-N16	102.12	C1-N16-O17-H30	-176.41
N16-O17	1.408	O17-N16-C1	112.86	C13-C14-C15-C10	0.40
C15-H29	1.083	H29-C15-C14	119.76	C13-C14-C15-H29	179.23
C14-H28	1.084	H29-C15-C10	119.70	H28-C14-C15-C10	-179.28
C14-C15	1.390	C14-C15-C10	120.53	H28-C14-C15-H29	-0.45

C13-H27	1.084	H28-C14-C15	119.71	C12-C13-C14-C15	-0.32
C13-C14	1.392	H28-C14-C13	120.09	C12-C13-C14-H28	179.36
C12-H26	1.084	C15-C14-C13	120.20	H27-C13-C14-C15	179.72
C12-C13	1.391	H27-C13-C14	120.14	H27-C13-C14-H28	-0.61
C11-H25	1.082	H27-C13-C12	120.20	C11-C12-C13-C14	0.01
C11-C12	1.390	C14-C13-C12	119.66	C11-C12-C13-H27	179.97
C10-C15	1.398	H26-C12-C13	120.08	H26-C12-C13-C14	179.92
C10-C11	1.397	H26-C12-C11	119.72	H26-C12-C13-H27	-0.12
C9-H24	1.082	C13-C12-C11	120.20	C10-C11-C12-C13	0.22
C8-H23	1.082	H25-C11-C12	120.38	C10-C11-C12-H26	-179.69
C8-C9	1.385	H25-C11-C10	119.05	H25-C11-C12-C13	-179.70
C7-Cl18	1.755	C12-C11-C10	120.57	H25-C11-C12-H26	0.40
C7-C8	1.391	C15-C10-C11	118.85	C1-C10-C15-C14	178.20
C6-H22	1.082	C15-C10-C1	121.03	C1-C10-C15-H29	-0.63
C6-C7	1.387	C11-C10-C1	120.10	C11-C10-C15-C14	-0.17
C5-H21	1.084	H24-C9-C8	118.55	C11-C10-C15-H29	-179.00
C5-C6	1.388	H24-C9-C4	120.17	C1-C10-C11-C12	-178.53
C4-C9	1.404	C8-C9-C4	121.28	C1-C10-C11-H25	1.39
C4-C5	1.402	H23-C8-C9	120.59	C15-C10-C11-C12	-0.14
C3-H20	1.085	H23-C8-C7	119.95	C15-C10-C11-H25	179.78
C3-C4	1.462	C9-C8-C7	119.46	C7-C8-C9-C4	-0.01
C2-H19	1.082	Cl18-C7-C8	119.48	C7-C8-C9-H24	179.85
C2-C3	1.344	Cl18-C7-C6	119.65	H23-C8-C9-C4	-179.97
C1-N16	1.290	C8-C7-C6	120.86	H23-C8-C9-H24	-0.11
C1-C10	1.490	H22-C6-C7	120.21	C6-C7-C8-C9	-0.05
C1-C2	1.460	H22-C6-C5	120.76	C6-C7-C8-H23	179.90
		C7-C6-C5	119.03	Cl18-C7-C8-C9	-179.97
		H21-C5-C6	119.06	Cl18-C7-C8-H23	-0.02
		H21-C5-C4	119.23	C5-C6-C7-C8	0.01
		C6-C5-C4	121.70	C5-C6-C7-Cl18	179.93
		C9-C4-C5	117.67	H22-C6-C7-C8	-180.00
		C9-C4-C3	123.59	H22-C6-C7-Cl18	-0.08
		C5-C4-C3	118.74	C4-C5-C6-C7	0.11
		H20-C3-C4	114.71	C4-C5-C6-H22	-179.88
		H20-C3-C2	118.47	H21-C5-C6-C7	179.95
		C4-C3-C2	126.82	H21-C5-C6-H22	-0.04
		H19-C2-C3	120.48	C3-C4-C9-C8	-179.87
		H19-C2-C1	114.92	C3-C4-C9-H24	0.27
		C3-C2-C1	124.55	C5-C4-C9-C8	0.12
		N16-C1-C10	114.27	C5-C4-C9-H24	-179.73
		N16-C1-C2	123.59	C3-C4-C5-C6	179.82
		C10-C1-C2	122.14	C3-C4-C5-H21	-0.02
				C9-C4-C5-C6	-0.17
				C9-C4-C5-H21	179.99
				C2-C3-C4-C5	-176.87
				C2-C3-C4-C9	3.12
				H20-C3-C4-C5	2.15
				H20-C3-C4-C9	-177.86
				C1-C2-C3-C4	178.82
				C1-C2-C3-H20	-0.17
				H19-C2-C3-C4	1.39
				H19-C2-C3-H20	-177.60
				C2-C1-N16-O17	2.28
				C10-C1-N16-O17	-177.50
				C2-C1-C10-C11	-130.91
				C2-C1-C10-C15	50.74
				N16-C1-C10-C11	48.88
				N16-C1-C10-C15	-129.48
				C10-C1-C2-C3	15.86
				C10-C1-C2-H19	-166.58
				N16-C1-C2-C3	-163.91
				N16-C1-C2-H19	13.65

Table B.3. Calculated Bond Lengths, Bond Angels and Dihedral Angles for Compound (*Z*)-4

Atoms	Bond Length	Atoms	Bond Angle	Atoms	Dihedral Angle
O17-H30	0.965	H30-O17-N16	102.41	C1-N16-O17-H30	178.86
N16-O17	1.399	O17-N16-C1	112.87	C13-C14-C15-C10	0.48
C15-H29	1.084	H29-C15-C14	119.99	C13-C14-C15-H29	-179.93
C14-H28	1.084	H29-C15-C10	119.64	H28-C14-C15-C10	-179.53
C14-C15	1.391	C14-C15-C10	120.37	H28-C14-C15-H29	0.06
C13-H27	1.083	H28-C14-C15	119.75	C12-C13-C14-C15	-0.27
C13-C14	1.391	H28-C14-C13	120.14	C12-C13-C14-H28	179.74
C12-H26	1.084	C15-C14-C13	120.11	H27-C13-C14-C15	179.81
C12-C13	1.391	H27-C13-C14	120.11	H27-C13-C14-H28	-0.18
C11-H25	1.083	H27-C13-C12	120.12	C11-C12-C13-C14	-0.17
C11-C12	1.390	C14-C13-C12	119.77	C11-C12-C13-H27	179.76

C10-C15	1.396	H26-C12-C13	120.09	H26-C12-C13-C14	-179.95
C10-C11	1.396	H26-C12-C11	119.73	H26-C12-C13-H27	-0.03
C9-H24	1.083	C13-C12-C11	120.18	C10-C11-C12-C13	0.40
C8-H23	1.082	H25-C11-C12	120.10	C10-C11-C12-H26	-179.82
C8-C9	1.385	H25-C11-C10	119.57	H25-C11-C12-C13	-179.38
C7-Cl18	1.755	C12-C11-C10	120.33	H25-C11-C12-H26	0.40
C7-C8	1.391	C15-C10-C11	119.25	C1-C10-C15-C14	-179.95
C6-H22	1.082	C15-C10-C1	120.24	C1-C10-C15-H29	0.46
C6-C7	1.387	C11-C10-C1	120.51	C11-C10-C15-C14	-0.24
C5-H21	1.084	H24-C9-C8	118.48	C11-C10-C15-H29	-179.84
C5-C6	1.388	H24-C9-C4	120.17	C1-C10-C11-C12	179.51
C4-C9	1.404	C8-C9-C4	121.35	C1-C10-C11-H25	-0.71
C4-C5	1.402	H23-C8-C9	120.57	C15-C10-C11-C12	-0.19
C3-H20	1.085	H23-C8-C7	119.96	C15-C10-C11-H25	179.59
C3-C4	1.462	C9-C8-C7	119.47	C7-C8-C9-C4	-0.04
C2-H19	1.085	Cl18-C7-C8	119.50	C7-C8-C9-H24	179.78
C2-C3	1.344	Cl18-C7-C6	119.69	H23-C8-C9-C4	-179.96
C1-N16	1.289	C8-C7-C6	120.81	H23-C8-C9-H24	-0.13
C1-C10	1.492	H22-C6-C7	120.21	C6-C7-C8-C9	-0.06
C1-C2	1.457	H22-C6-C5	120.73	C6-C7-C8-H23	179.86
		C7-C6-C5	119.07	Cl18-C7-C8-C9	-179.96
		H21-C5-C6	119.04	Cl18-C7-C8-H23	-0.04
		H21-C5-C4	119.22	C5-C6-C7-C8	0.04
		C6-C5-C4	121.75	C5-C6-C7-Cl18	179.94
		C9-C4-C5	117.56	H22-C6-C7-C8	-179.95
		C9-C4-C3	123.64	H22-C6-C7-Cl18	-0.04
		C5-C4-C3	118.80	C4-C5-C6-C7	0.08
		H20-C3-C4	114.97	C4-C5-C6-H22	-179.93
		H20-C3-C2	118.16	H21-C5-C6-C7	179.97
		C4-C3-C2	126.87	H21-C5-C6-H22	-0.05
		H19-C2-C3	121.20	C3-C4-C9-C8	-179.87
		H19-C2-C1	113.95	C3-C4-C9-H24	0.31
		C3-C2-C1	124.85	C5-C4-C9-C8	0.16
		N16-C1-C10	124.00	C5-C4-C9-H24	-179.67
		N16-C1-C2	114.61	C3-C4-C5-C6	179.85
		C10-C1-C2	121.40	C3-C4-C5-H21	-0.04
				C9-C4-C5-C6	-0.18
				C9-C4-C5-H21	179.94
				C2-C3-C4-C5	-177.68
				C2-C3-C4-C9	2.35
				H20-C3-C4-C5	1.97
				H20-C3-C4-C9	-178.00
				C1-C2-C3-C4	179.64
				C1-C2-C3-H20	0.00
				H19-C2-C3-C4	0.49
				H19-C2-C3-H20	-179.15
				C2-C1-N16-O17	-179.62
				C10-C1-N16-O17	0.47
				C2-C1-C10-C11	-106.31
				C2-C1-C10-C15	73.39
				N16-C1-C10-C11	73.60
				N16-C1-C10-C15	-106.70
				C10-C1-C2-C3	3.14
				C10-C1-C2-H19	-177.66
				N16-C1-C2-C3	-176.78
				N16-C1-C2-H19	2.42

Table B.4. Calculated Bond Lengths, Bond Angels and Dihedral Angles for Compound (*E*)-6a

Atoms	Bond Length	Atoms	Bond Angle	Atoms	Dihedral Angle
H43-C24	1.085	H43-C24-C19	119.484	C23-C24-C19-C20	0.17
H42-C23	1.084	H43-C24-C23	119.75	C23-C24-C19-C18	-178.867
H41-C22	1.084	C19-C24-C23	120.766	H43-C24-C19-C20	-179.712
H40-C21	1.084	H42-C23-C24	119.944	H43-C24-C19-C18	1.251
H39-C20	1.083	H42-C23-C22	120.117	C19-C24-C23-C22	0.006
H38-C18	1.091	C24-C23-C22	119.939	C19-C24-C23-H42	-179.781
H37-C18	1.091	H41-C22-C23	120.113	H43-C24-C23-C22	179.888
H36-C16	1.083	H41-C22-C21	120.121	H43-C24-C23-H42	0.101
H35-C15	1.082	C23-C22-C21	119.765	C24-C23-C22-C21	-0.098
H34-C13	1.082	H40-C21-C22	120.034	C24-C23-C22-H41	-179.852
H33-C12	1.084	H40-C21-C20	119.829	H42-C23-C22-C21	179.688
H32-C10	1.086	C22-C21-C20	120.138	H42-C23-C22-H41	-0.065
H31-C9	1.082	H39-C20-C21	120.068	C23-C22-C21-C20	0.011
H30-C8	1.084	H39-C20-C19	119.374	C23-C22-C21-H40	-179.841
H29-C7	1.084	C21-C20-C19	120.555	H41-C22-C21-C20	179.765
H28-C6	1.084	C18-C19-C24	120.376	H41-C22-C21-H40	-0.087
H27-C5	1.083	C18-C19-C20	120.78	C22-C21-C20-C19	0.169

H26-C1	1.082	C24-C19-C20	118.837	C22-C21-C20-H39	179.585
Cl25-C14	1.755	H37-C18-H38	109.155	H40-C21-C20-C19	-179.979
C24-C19	1.396	H37-C18-O17	108.233	H40-C21-C20-H39	-0.562
C24-C23	1.391	H37-C18-C19	111.407	C21-C20-C19-C24	-0.257
C23-C22	1.391	H38-C18-O17	103.91	C21-C20-C19-C18	178.776
C22-C21	1.392	H38-C18-C19	110.768	H39-C20-C19-C24	-179.678
C21-C20	1.391	O17-C18-C19	113.048	H39-C20-C19-C18	-0.645
C20-C19	1.396	N3-O17-C18	109.462	C20-C19-C18-O17	-88.957
C19-C18	1.507	H36-C16-C11	120.135	C20-C19-C18-H38	154.892
C18-O17	1.441	H36-C16-C15	118.572	C20-C19-C18-H37	33.184
O17-N3	1.396	C11-C16-C15	121.293	C24-C19-C18-O17	90.061
C16-C11	1.404	H35-C15-C16	120.585	C24-C19-C18-H38	-26.09
C16-C15	1.385	H35-C15-C14	119.949	C24-C19-C18-H37	-147.798
C15-C14	1.391	C16-C15-C14	119.466	C19-C18-O17-N3	81.315
C14-C13	1.387	Cl25-C14-C15	119.479	H38-C18-O17-N3	-158.529
C13-C12	1.388	Cl25-C14-C13	119.672	H37-C18-O17-N3	-42.586
C12-C11	1.402	C15-C14-C13	120.85	C18-O17-N3-C2	-170.543
C11-C10	1.462	H34-C13-C14	120.213	C15-C16-C11-C12	0.245
C10-C1	1.344	H34-C13-C12	120.754	C15-C16-C11-C10	-179.86
C9-C8	1.390	C14-C13-C12	119.033	H36-C16-C11-C12	-179.465
C9-C4	1.398	H33-C12-C13	119.053	H36-C16-C11-C10	0.43
C8-C7	1.391	H33-C12-C11	119.231	C11-C16-C15-C14	-0.035
C7-C6	1.392	C13-C12-C11	121.716	C11-C16-C15-H35	-179.922
C6-C5	1.390	C10-C11-C16	123.553	H36-C16-C15-C14	179.68
C5-C4	1.399	C10-C11-C12	118.805	H36-C16-C15-H35	-0.207
C4-C2	1.490	C16-C11-C12	117.642	C16-C15-C14-C13	-0.114
N3-C2	1.292	H32-C10-C1	118.457	C16-C15-C14-Cl25	-179.988
C2-C1	1.460	H32-C10-C11	114.726	H35-C15-C14-C13	179.773
		C1-C10-C11	126.807	H35-C15-C14-Cl25	-0.101
		H31-C9-C8	120.383	C15-C14-C13-C12	0.043
		H31-C9-C4	119.018	C15-C14-C13-H34	-179.903
		C8-C9-C4	120.599	Cl25-C14-C13-C12	179.917
		H30-C8-C9	119.723	Cl25-C14-C13-H34	-0.03
		H30-C8-C7	120.076	C14-C13-C12-C11	0.179
		C9-C8-C7	120.2	C14-C13-C12-H33	179.996
		H29-C7-C8	120.203	H34-C13-C12-C11	-179.874
		H29-C7-C6	120.154	H34-C13-C12-H33	-0.058
		C8-C7-C6	119.643	C13-C12-C11-C16	-0.319
		H28-C6-C7	120.096	C13-C12-C11-C10	179.781
		H28-C6-C5	119.693	H33-C12-C11-C16	179.865
		C7-C6-C5	120.21	H33-C12-C11-C10	-0.035
		H27-C5-C6	119.787	C12-C11-C10-C1	-175.145
		H27-C5-C4	119.646	C12-C11-C10-H32	3.698
		C6-C5-C4	120.556	C16-C11-C10-C1	4.961
		C2-C4-C9	120.146	C16-C11-C10-H32	-176.196
		C2-C4-C5	121.04	C11-C10-C1-C2	179.104
		C9-C4-C5	118.79	C11-C10-C1-H26	1.724
		C2-N3-O17	113.171	H32-C10-C1-C2	0.299
		C1-C2-N3	123.597	H32-C10-C1-H26	-177.081
		C1-C2-C4	122.058	C4-C9-C8-C7	0.195
		N3-C2-C4	114.346	C4-C9-C8-H30	-179.663
		H26-C1-C2	114.822	H31-C9-C8-C7	-179.835
		H26-C1-C10	120.533	H31-C9-C8-H30	0.306
		C2-C1-C10	124.599	C8-C9-C4-C5	-0.04
				C8-C9-C4-C2	-178.286
				H31-C9-C4-C5	179.99
				H31-C9-C4-C2	1.744
				C9-C8-C7-C6	-0.045
				C9-C8-C7-H29	179.963
				H30-C8-C7-C6	179.813
				H30-C8-C7-H29	-0.179
				C8-C7-C6-C5	-0.261
				C8-C7-C6-H28	179.372
				H29-C7-C6-C5	179.732
				H29-C7-C6-H28	-0.635
				C7-C6-C5-C4	0.419
				C7-C6-C5-H27	179.249
				H28-C6-C5-C4	-179.216
				H28-C6-C5-H27	-0.385
				C6-C5-C4-C9	-0.266
				C6-C5-C4-C2	177.964
				H27-C5-C4-C9	-179.098
				H27-C5-C4-C2	-0.869
				C5-C4-C2-N3	-130.991
				C5-C4-C2-C1	49.019
				C9-C4-C2-N3	47.215

C9-C4-C2-C1	-132.775
O17-N3-C2-C4	-176.022
O17-N3-C2-C1	3.967
C4-C2-C1-C10	18.245
C4-C2-C1-H26	-164.241
N3-C2-C1-C10	-161.743
N3-C2-C1-H26	15.771

Table B.5. Calculated Bond Lengths, Bond Angels and Dihedral Angles for Compound (*Z*)-6a

Atoms	Bond Length	Atoms	Bond Angle	Atoms	Dihedral Angle
H43-C24	1.083	H43-C24-C14	119.371	C23-C24-C14-C20	0.34
H42-C23	1.084	H43-C24-C23	120.051	C23-C24-C14-C13	-178.423
H41-C22	1.084	C14-C24-C23	120.576	H43-C24-C14-C20	179.762
H40-C21	1.084	H42-C23-C24	119.835	H43-C24-C14-C13	0.999
H39-C20	1.085	H42-C23-C22	120.032	C14-C24-C23-C22	-0.216
H38-C19	1.083	C24-C23-C22	120.133	C14-C24-C23-H42	179.967
H37-C18	1.082	H41-C22-C23	120.131	H43-C24-C23-C22	-179.633
H36-C16	1.082	H41-C22-C21	120.116	H43-C24-C23-H42	0.549
H35-C15	1.084	C23-C22-C21	119.753	C24-C23-C22-C21	-0.029
H34-C13	1.092	H40-C21-C22	120.109	C24-C23-C22-H41	-179.765
H33-C13	1.091	H40-C21-C20	119.929	H42-C23-C22-C21	179.789
H32-C10	1.085	C22-C21-C20	119.961	H42-C23-C22-H41	0.052
H31-C8	1.085	H39-C20-C21	119.76	C23-C22-C21-C20	0.142
H30-C6	1.081	H39-C20-C14	119.486	C23-C22-C21-H40	-179.645
H29-C4	1.084	C21-C20-C14	120.754	H41-C22-C21-C20	179.879
H28-C3	1.084	H38-C19-C11	120.084	H41-C22-C21-H40	0.091
H27-C2	1.084	H38-C19-C18	118.559	C22-C21-C20-C14	-0.013
H26-C1	1.084	C11-C19-C18	121.352	C22-C21-C20-H39	-179.917
Cl25-C17	1.756	H37-C18-C19	120.605	H40-C21-C20-C14	179.775
C24-C14	1.396	H37-C18-C17	119.953	H40-C21-C20-H39	-0.129
C24-C23	1.390	C19-C18-C17	119.44	C21-C20-C14-C24	-0.226
C23-C22	1.392	Cl25-C17-C18	119.49	C21-C20-C14-C13	178.543
C22-C21	1.391	Cl25-C17-C16	119.678	H39-C20-C14-C24	179.678
C21-C20	1.391	C18-C17-C16	120.831	H39-C20-C14-C13	-1.553
C20-C14	1.396	H36-C16-C17	120.197	C18-C19-C11-C15	-0.796
C19-C11	1.404	H36-C16-C15	120.739	C18-C19-C11-C10	179.284
C19-C18	1.385	C17-C16-C15	119.064	H38-C19-C11-C15	178.431
C18-C17	1.391	H35-C15-C16	119.084	H38-C19-C11-C10	-1.489
C17-C16	1.387	H35-C15-C11	119.189	C11-C19-C18-C17	0.319
C16-C15	1.388	C16-C15-C11	121.727	C11-C19-C18-H37	179.824
C15-C11	1.402	C13-C14-C24	120.815	H38-C19-C18-C17	-178.92
C14-C13	1.507	C13-C14-C20	120.351	H38-C19-C18-H37	0.586
C13-O12	1.441	C24-C14-C20	118.822	C19-C18-C17-C16	0.229
O12-N9	1.393	H33-C13-H34	109.174	C19-C18-C17-Cl25	179.837
C11-C10	1.462	H33-C13-O12	103.964	H37-C18-C17-C16	-179.28
C10-C8	1.342	H33-C13-C14	110.748	H37-C18-C17-Cl25	0.328
N9-C7	1.289	H34-C13-O12	108.332	C18-C17-C16-C15	-0.265
C8-C7	1.471	H34-C13-C14	111.501	C18-C17-C16-H36	179.669
C7-C5	1.490	O12-C13-C14	112.803	Cl25-C17-C16-C15	-179.873
C6-C1	1.389	N9-O12-C13	109.551	Cl25-C17-C16-H36	0.061
C6-C5	1.399	C10-C11-C19	123.525	C17-C16-C15-C11	-0.245
C5-C4	1.398	C10-C11-C15	118.895	C17-C16-C15-H35	-179.95
C4-C3	1.390	C19-C11-C15	117.58	H36-C16-C15-C11	179.822
C3-C2	1.390	H32-C10-C8	117.505	H36-C16-C15-H35	0.116
C2-C1	1.392	H32-C10-C11	115.58	C16-C15-C11-C19	0.761
		C8-C10-C11	126.909	C16-C15-C11-C10	-179.315
		C7-N9-O12	113.864	H35-C15-C11-C19	-179.534
		H31-C8-C7	114.984	H35-C15-C11-C10	0.39
		H31-C8-C10	120.385	C20-C14-C13-O12	-91.121
		C7-C8-C10	124.617	C20-C14-C13-H34	146.716
		C5-C7-C8	117.55	C20-C14-C13-H33	24.932
		C5-C7-N9	126.291	C24-C14-C13-O12	87.623
		C8-C7-N9	116.159	C24-C14-C13-H34	-34.539
		H30-C6-C1	120.005	C24-C14-C13-H33	-156.324
		H30-C6-C5	119.593	C14-C13-O12-N9	-82.957
		C1-C6-C5	120.401	H34-C13-O12-N9	40.971
		C7-C5-C6	121.825	H33-C13-O12-N9	157.007
		C7-C5-C4	119.365	C13-O12-N9-C7	172.551
		C6-C5-C4	118.762	C15-C11-C10-C8	169.754
		H29-C4-C5	119.539	C15-C11-C10-H32	-9.335
		H29-C4-C3	119.704	C19-C11-C10-C8	-10.327
		C5-C4-C3	120.753	C19-C11-C10-H32	170.584
		H28-C3-C4	119.778	C11-C10-C8-C7	178.179
		H28-C3-C2	120.203	C11-C10-C8-H31	-3.238
		C4-C3-C2	120.018	H32-C10-C8-C7	-2.748

H27-C2-C3	120.18	H32-C10-C8-H31	175.836
H27-C2-C1	120.161	O12-N9-C7-C8	174.362
C3-C2-C1	119.658	O12-N9-C7-C5	-5.809
H26-C1-C6	119.6	C10-C8-C7-N9	-28.054
H26-C1-C2	120.003	C10-C8-C7-C5	152.101
C6-C1-C2	120.397	H31-C8-C7-N9	153.295
		H31-C8-C7-C5	-26.55
		N9-C7-C5-C4	135.751
		N9-C7-C5-C6	-46.807
		C8-C7-C5-C4	-44.421
		C8-C7-C5-C6	133.02
		C5-C6-C1-C2	-0.788
		C5-C6-C1-H26	179.352
		H30-C6-C1-C2	179.493
		H30-C6-C1-H26	-0.367
		C1-C6-C5-C4	0.065
		C1-C6-C5-C7	-177.392
		H30-C6-C5-C4	179.785
		H30-C6-C5-C7	2.329
		C6-C5-C4-C3	0.853
		C6-C5-C4-H29	-179.872
		C7-C5-C4-C3	178.373
		C7-C5-C4-H29	-2.352
		C5-C4-C3-C2	-1.05
		C5-C4-C3-H28	179.188
		H29-C4-C3-C2	179.676
		H29-C4-C3-H28	-0.086
		C4-C3-C2-C1	0.318
		C4-C3-C2-H27	-179.52
		H28-C3-C2-C1	-179.92
		H28-C3-C2-H27	0.241
		C3-C2-C1-C6	0.595
		C3-C2-C1-H26	-179.545
		H27-C2-C1-C6	-179.566
		H27-C2-C1-H26	0.294