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Structural isomers of 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one: A Theoretical Study

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ABSTRACT

A series of 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one molecules were theoretically investigated by the use of density functional theory (DFT) calculations at the B3LYP/6-311++G** level of the theory. The substituents studied in this work are X = H; CH_3; NH_2; OH; OCH_3; F, Cl; Br; NO_2; CN; $COCH_3$; CO_2H; CO_2Me; SH; BH_2. We have selected these functional groups to be placed in the 2, 3 and 4 positions with relation to the benzisoselenazol moiety in order to show the effect of these structural modifications on the electronic properties of the molecules.

1. Introduction

The development in organoselenium chemistry has been expanding rapidly over the last several years. In spite of the odor problem, there is a remarkable level of interest (among chemists and biochemists) in organoselenium compounds which are apparent from literature surveys. This has been increasing particularly with the growing recognition of their key roles in biological processes especially as possible anti-carcinogens [1–3]. Many investigative reports have been demonstrated that organoselenium compounds are less toxic than those of inorganic selenium compounds. Thus, there is interest in the synthesis and investigation of novel organoselenium compounds for their use in enzymology and bioorganic chemistry [4–10].

Selenium has been recognized as an essential component of the active site for several enzymes since it is present in the selenocyteine and selenomethionine amino acid derivations. Four glutathione peroxidases (among them cytosolic glutathione peroxidase which is the first established selenoenzyme) protect cells against peroxidative damage by reducing hydrogen peroxide, free fatty acid hydroperoxides, and phospholipids hydroperoxides [11–15] and is related to these species being discussed. Studies even up to seventeen years old depict that the heterocyclic compounds of selenium such as selenirenes, selenophenes, selenadiazoles, selenatriazoles and benzisoselanazolones can have various biological effects. Among such characteristics they are active immunostimulants, inhibitors of enzymes, antioxidants, anti-inflammatory, antitumor, antiviral and antimicrobial agents [16].

Various organoselenium compounds having a direct Se–N bond have been shown to mimic the active site of GPx. Among such systems is the most promising drug labeled as the Ebselen molecule class [17]. The Ebselen molecule (2-phenyl-1,2-benzisoselenazol-3(2H)-one) was first reported in 1924 by Lesser and Weiss [18]. The most useful experimental method was reported by Engman in 1989 [19]. Since the laboratory creation of this molecule, several competing synthetic methodologies have been developed to functionalize the Ebselen with different group to test them as potential pharmaceuticals [20,21]. Ebselen and its derivatives are re-known for their numerous pharmacological activities, especially as free radical scavengers. These abilities can be attributed to their selenocontaining structure with glutathione peroxidase like activity [22–26].

Several clinical trials deal with Ebselen species and have demonstrated promising results for use as novel antioxidants [27]. Theoretical modeling of these systems or other selenoproteins has been relatively underutilized [28–30]. Today the B3LYP variant of DFT calculations is the method of choice for most investigators working on practical theoretical problems of oxidative chemistry. Direct comparison of B3LYP data with that of other methods by a number of investigators has proven its general applicability.

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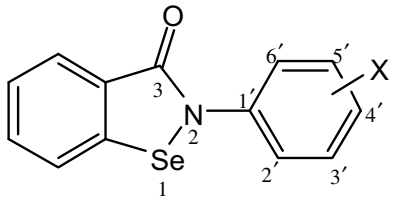


Scheme 1. General representations of the 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one structures where X = H; CH_3;NH_2; OH; OCH_3; F, Cl; Br; NO_2; CN; $COCH_3$; CO_2H; CO_2Me; SH; BH_2.

The present work focuses on the study of the structural and electronic properties of Ebselen (2-phenyl-1,2-benzisoselenazol-3(2H)-one) and its derivatives of 2-(2,3 and 4-substituted)-phenyl-1,2-benzisoselenazol-3(2H)-one (see Scheme 1) . This has been approached by DFT methods in order to support the physical role of organoselenium compounds.

2. Computational methods

The quantum chemical calculations in this work were performed with the GAUSSIAN03 program codes [31]. Geometry optimizations were performed with the Density Functional Theory (DFT)-B3LYP method coupled to the 6-311++G** basis set. Higher level calculations require vast computational limitations, but since it is our goal to provide general trends this method should suffice. Tight convergence criteria were applied to make sure that the energies obtained were accurate enough within the realm of the methods employed for which further information is elsewhere available [32].

3. Results and discussion

3.1. Geometrical characteristics

Scheme 1 denotes the basic structure of the molecules under consideration with the substituents used also displayed. It is important to note that the structures optimized are minimum energy species which have been studied by multiple torsional potential analysis. In other words, many competing structures were computed but only the lowest energy species have been presented for each configuration (*ortho*, *meta* and *para*) for reasons of practicality.

Table 1 listed some of selected structural parameters (bond length, angles and dihedral angles) of the optimized geometries. As shown in this table, there is no obvious trend for the variation of these parameters. The values of the bond length and angles of

Table 1
Selected structural parameters (bond lengths, bond angle and dihedral angles) of the 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one structures where X = H; CH_3; NH_2; OH; OCH_3; F, Cl; Br; NO_2; CN; $COCH_3$; CO_2H; CO_2Me; SH; BH_2

X	H	CH_3	NH_2	OH	SH	OCH_3	F	Cl	Br	NO_2	CN	CO_2H	CO_2CH_3	BH_2
Ortho series														
Bond distance (Å)														
Se–N	1.909	1.924	1.919	1.918	1.901	1.904	1.927	1.937	1.938	1.899	1.930	1.964	1.898	1.897
C3–N	1.399	1.413	1.408	1.408	1.384	1.392	1.407	1.415	1.417	1.395	1.417	1.436	1.395	1.390
C=O	1.221	1.221	1.222	1.220	1.225	1.220	1.221	1.221	1.221	1.217	1.219	1.221	1.217	1.220
N–C1′	1.421	1.447	1.450	1.443	1.384	1.423	1.421	1.429	1.429	1.395	1.419	1.438	1.423	1.427
Bond angles (°)														
C3–N–Se	114.07	111.48	111.48	111.80	115.26	115.36	113.20	112.00	111.85	115.88	112.58	110.12	115.63	115.65
Se–N–C1′	119.09	122.96	122.92	122.46	119.21	119.99	121.99	123.48	123.59	121.37	122.37	126.31	121.29	120.10
C3–N–C1′	126.84	125.56	125.60	125.74	125.47	123.79	124.80	124.51	124.56	122.73	125.06	123.56	123.08	123.78
Dihedral angles (°)														
Se–N–C1′–C2′	0.00	0.00	0.00	0.00	−60.36	−70.69	0.00	0.00	0.00	69.08	0.00	0.00	69.34	−107.35
C3–N–C1′–C6′	0.00	0.00	0.00	0.00	−65.40	−69.32	0.00	0.00	0.00	72.18	0.00	0.00	68.39	−116.30
Meta series														
Bond distance (Å)														
Se–N	–	1.909	1.909	1.909	1.910	1.910	1.909	1.910	1.910	1.912	1.911	1.912	1.911	1.900
C3–N	–	1.400	1.400	1.400	1.401	1.400	1.402	1.401	1.402	1.403	1.403	1.402	1.400	1.395
C=O	–	1.221	1.220	1.220	1.220	1.220	1.219	1.220	1.229	1.220	1.220	1.220	1.220	1.220
N–C1′	–	1.422	1.423	1.421	1.419	1.422	1.418	1.418	1.418	1.414	1.415	1.415	1.416	1.421
Bond angles (°)														
C3–N–Se	–	114.05	113.97	113.97	113.97	113.96	114.07	114.04	114.06	114.17	114.06	114.2	114.26	115.20
Se–N–C1′	–	119.14	119.12	119.29	119.32	119.27	119.23	119.32	119.31	119.25	119.37	119.14	119.06	119.82
C3–N–C1′	–	126.82	126.91	126.74	126.71	127.77	126.69	126.64	126.64	126.57	126.57	126.65	126.68	124.98
Dihedral angles (°)														
Se–N–C1′–C2′	–	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	38.94
C3–N–C1′–C6′	–	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	39.76
Para series														
Bond distance (Å)														
Se–N	–	1.909	1.907	1.908	1.909	1.908	1.909	1.910	1.910	1.913	1.911	1.912	1.912	1.907
C3–N	–	1.397	1.393	1.396	1.398	1.396	1.398	1.399	1.400	1.408	1.406	1.405	1.403	1.403
C=O	–	1.221	1.223	1.222	1.221	1.222	1.221	1.221	1.220	1.218	1.219	1.219	1.219	1.218
N–C1′	–	1.421	1.426	1.423	1.420	1.423	1.421	1.418	1.418	1.409	1.412	1.413	1.414	1.413
Bond angles (°)														
C3–N–Se	–	114.13	114.20	114.16	114.14	114.18	114.11	114.09	114.09	113.93	113.97	113.96	113.98	114.62
Se–N–C1′	–	119.01	118.99	119.07	119.13	118.99	119.22	119.23	119.25	119.45	119.40	119.29	119.22	119.42
C3–N–C1′	–	126.86	126.80	126.77	126.73	126.83	126.67	126.68	126.66	126.62	126.63	126.75	126.80	125.96
Dihedral angles (°)														
Se–N–C1′–C2′	–	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3–N–C1′–C6′	–	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 2
Relative energies (ΔE) and free energies (ΔG) in kcal/mol where 0 K is the sum of zero-point and electronic energies

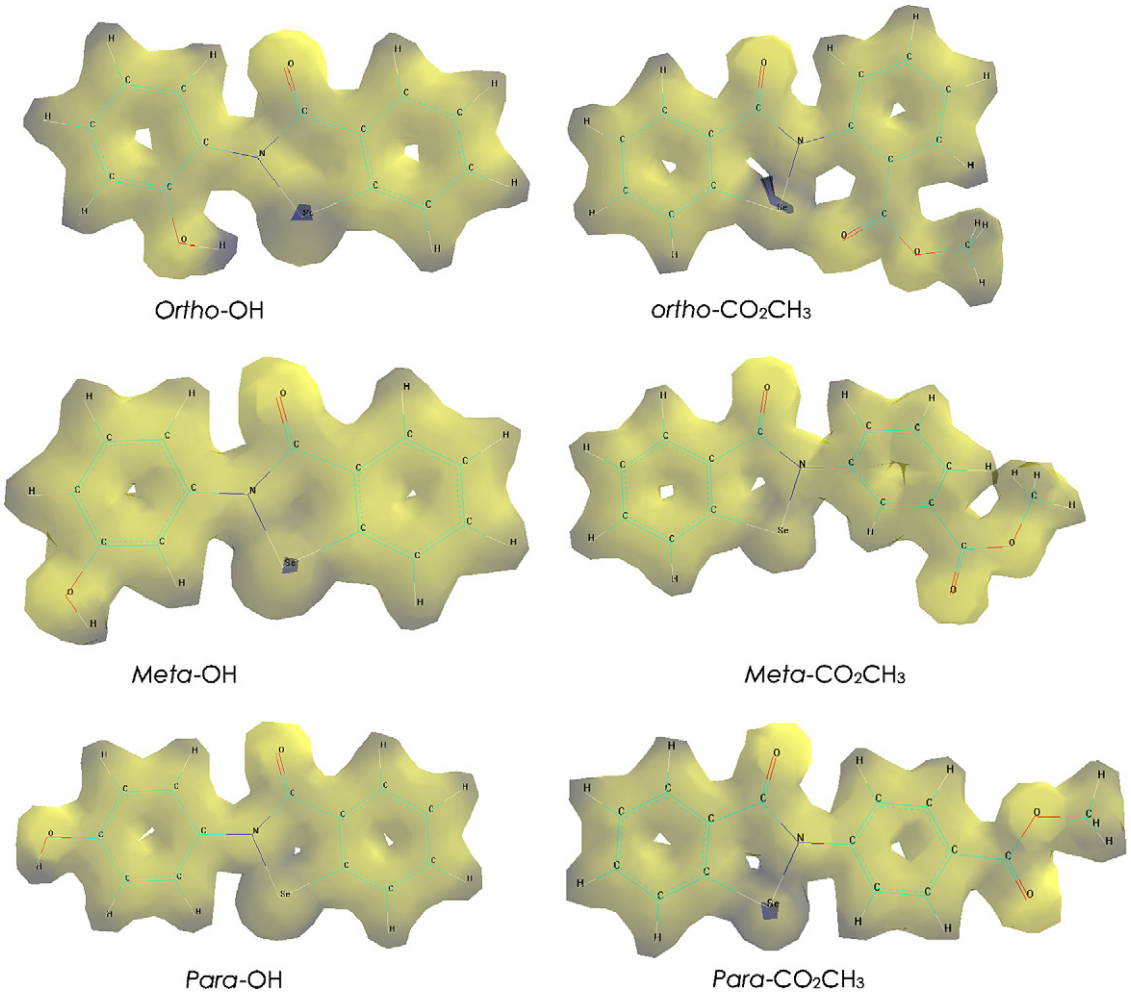
Substituent	ΔG			ΔE			ΔE (0 K)		
X	*Ortho*	*Meta*	*Para*	*Ortho*	*Meta*	*Para*	*Ortho*	*Meta*	*Para*
CH_3	13.83	0.00	0.06	13.63	0.00	0.02	13.83	0.00	0.05
NH_2	13.53	0.00	0.24	13.45	0.00	0.35	13.20	0.00	0.35
OH	12.03	0.00	0.27	12.14	0.00	0.24	11.81	0.00	0.32
SH	1.86	0.00	0.34	1.32	0.00	0.14	0.61	0.00	0.15
OCH_3	2.00	0.00	0.01	2.76	0.00	0.24	2.53	0.00	0.23
F	3.75	0.00	0.34	3.42	0.00	0.42	3.53	0.00	0.44
Cl	9.52	0.26	0.00	9.22	0.06	0.00	9.17	0.07	0.00
Br	11.15	0.40	0.00	10.83	0.09	0.00	10.75	0.11	0.00
NO_2	6.14	1.08	0.00	7.63	0.93	0.00	7.55	0.90	0.00
CN	7.30	1.10	0.00	6.99	0.93	0.00	6.94	0.92	0.00
$COCH_3$	14.06	16.70	0.00	16.22	15.72	0.00	15.70	15.55	0.00
CO_2H	28.22	7.71	0.00	27.37	7.38	0.00	26.38	6.79	0.00
BH_2	2.82	0.72	0.00	3.33	0.90	0.00	3.24	0.85	0.00

the optimized geometries are quite similar. The values shown are unaffected by the change in the type and position of chemical group in the phenyl ring. The dihedral angles of Se–N–C1′–C2′ and C3–N–C1′–C6′ angles for most of the presented molecules yielded values close to 0.00. This represents that the geometry optimization of the studied molecules at the B3LYP/6-311++G** level yield planar structures for these geometries. In contrast, the geometry optimization of the (*ortho* OCH_3, SH, CO_2CH_3 and BH_2) isomers and *meta* BH_2 isomer at the same level of theory yield non-planar structures. The geometrical parameters are important to include for the connection of energetic parameters to physical properties. They serve as guides for future data basing of such geometrical parameters in experimental corroboration of our calculated findings.

In the supporting information of this work we present a scheme that graphical depicts the nature of various vibrational frequencies for these molecules. In this scheme, we have listed in Tables S1–S2 of the supporting information for which a few vibrational modes (in cm^{-1}) where v_1 and v_2 = stretching, v_3 = asymmetrical stretching, v_4 = breathing and v_5 is the functional group stretching mode (denoted as R) were provided. This can help experimentalists in trying to make theoretical comparisons for future analysis.

3.2. Thermodynamic properties

Table 2 displays the relative energies (ΔE) and free energies (ΔG) in kcal/mol for these species where 0 K is the sum of zero-point and electronic energies. The free energies have been calculated using molecular entropies in order to evaluate this effect on the relative stabilities. As previously mentioned, the first groups from CH_3 to F have the *meta* structure as the minimum energy species, whereas Cl to BH_2 have the *para* structure as the lowest energy configuration. In the first set of molecules, we can see that the ΔG values are 13.8, 13.5, 12.0, 1.9, 2.0 and 3.5 kcal/mol for H, CH_3, NH_2, OH, SH, OCH_3 and F, respectively. This is significantly larger than the corresponding computed values of 0.06, 0.24, 0.27,



Scheme 2. Three dimensions isosurface plots of the electrostatic potential for selected molecules.

0.34, 0.01 and 0.34 kcal/mol for H, CH_3, NH_2, OH, SH, OCH_3 and F, respectively, for the *para* configuration.

The ΔE values for such configurations are similar and the separations decrease with the implementation of zero-point corrections. It is clear that in the *ortho* isomer unfavorable interactions arise due to the proximity to the Se atom (which is accounted for by steric crowding). Interestingly, for several of the groups explored (especially NH_2, OH, SH and OCH_3) a strong non-covalent attraction with the Se and N atom is observed. This effect (which will be addressed later) consequently stabilizes the molecular structure.

For the next group of molecular species we obtain ΔG values of 9.52, 11.15, 6.14, 7.30, 14.06, 28.22 and 2.82 kcal/mol for the *ortho* configuration of Cl, Br, NO_2, CN, CO_2CH_3, CO_2H and BH_2, respectively. This is lower in comparison to the values of 0.26, 0.40, 1.08, 1.10, 16.70, 7.71 and 0.72 kcal/mol for the *meta* configuration of Cl, Br, NO_2, CN, CO_2CH_3, CO_2H and BH_2, respectively. In these structures, the molecular species have been stabilized by similar Se–N interactions as in the previous cases. The bulky nature of their composition causes the *para* configuration to be lower in energy. This can be explained by considering the degrees of freedom in this molecule which causes the energy to be reduced by allowing the functional groups to have reduced steric effects. The qualitative results are consistent in this group which allows us to make generalizations about their chemical reactivity.

3.3. Electrostatic potential isosurface

The three-dimensional mapped isosurface of the electrostatic potential for selected molecules (*ortho*, *meta* and *para* isomers of OH and CO_2CH_3) is shown in Scheme 2. This plot provides information on the reactivity of the molecules in actual reactions with electrophiles or nucleophiles. Dark (black) colors indicate positive ESP regions and light (yellow) colors indicate negative ESP regions.

In general for the isomers calculated, the plots show that the selenium atom has a positive ESP region. This suggests that the selenium atom can be more easily oxidized and reduced between valence state **II** and **IV**. The C-3 atom has a more positive ESP region, while the two phenyl rings gets less positive ESP regions. On the contrary, if we analyze the region of the oxygen atom we can see that the carbonyl group has a negative ESP region. This suggests that oxygen atom would probably undergo a protonation reaction with acidic reagents. Such conclusions are important in the understand of the physical properties for the molecules studied. Future calculations on the reactivity along these sites can be generated as a result of a careful analysis of the plots provided.

4. Conclusions

From this study we have explored multiple configurations of 2-(2,3 and 4-substituted-phenyl-1,2-benzisoselenazol)-3(2H)-one. The values of the bond length and angles of the optimized geometries are quite similar and maintain their configuration despite variations in the type and position of chemical group in the phenyl ring. Geometry optimization of most the studied molecules yield planar structures except for the *ortho* configurations of OCH_3, SH, CO_2CH_3 and BH_2 and *meta* BH_2 which were not planar. The calculations reveal that certain structures such as H, CH_3, NH_2, OH, SH, OCH_3 and F prefer the *meta* configuration whereas Cl, Br, NO_2, CN, CO_2CH_3, CO_2H and BH_2 prefer the *para* structures. This is due to the fact that the latter groups have bulky groups that need to have the amount of steric hindrance reduced.

To further evaluate the exact nature of the Se–C and the Se–N interactions existing within these structures calculations using the Bader theory of atoms in molecules (AIM) [33] has been applied. It is based on a topological analysis of the electronic charge density, ρ. The optimized geometries were employed to obtain wave function files suitable for use with AIM 2000, which suits the programs [34] and were applied to perform the AIM calculations.

From the calculations we observed that changing substitution in the *ortho* position caused that electron density at Se–C and Se–N bonds considerably changed. In this situation, the electron density at Se–C and Se–N bonds are minimum with X = NO_2 and X = CO_2H, respectively. On the other hand, the electron density at Se–C and Se–N bonds will be maximized with X = NH_2 and X = BH_2, respectively. The sample calculations reveal that the electron density does not affected by substitution in *meta* position because changes of resonance with change substitution in meta position does not affect on charge density of atom that linked to N atom. The same results were obtained with substituents in the *para* position, it must be mentioned that electron densities in this situation are closer together than before. The reason of this fact (except resonance effect) is also caused by the reduction of the inductive effect on the atoms linked to nitrogen. This serves to clarify the nature of the Se interactions with competing atoms of the complex.

Potentially such calculations are of importance in biochemistry whereby new complexes of Se are being used due to their capability to trap free radicals that prevents harmful damage to DNA and other biologically related molecules. This work should be of importance to workers in the field of novel molecules of biological interest in the gas phase.

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Special thanks are extended to DGSCA of the UNAM for valuable resources and to the University of Arizona for supercomputer time. Supporting information with vibrational frequencies of the studied molecules are available in the online version of this manuscript.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jorganchem.2008.02.026.

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