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A comprehensive account of spectral, Hartree Fock, and Density Functional Theory studies of 2-chlorobenzothiazole

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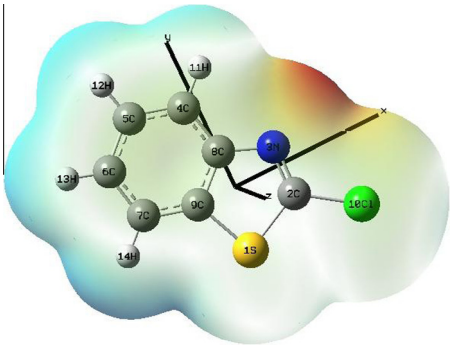
HIGHLIGHTS

- Corroboration of structure of 2CBT through comprehensive spectroscopic strategies.
- HF and DFT calculations to support structural findings of 2CBT.
- TDDFT approach undertaken to predict electronic properties.
- Electrostatic potential energy surfaces were analyzed.

GRAPHICAL ABSTRACT



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ABSTRACT

Benzothiazole moiety is found to play an important role in medicinal chemistry with a wide range of pharmacological activities. Herein, a simple, benzothiazole derivative *viz.*, 2-chlorobenzothiazole (2CBT) has been analyzed. The spectroscopic properties of the target compound were examined by FT-IR (4400–450 cm^{-1}), FT-Raman (4000–50 cm^{-1}), and NMR techniques. The ^{1}H and ^{13}C NMR spectra were recorded in DMSO. Theoretical calculations were performed by *ab initio* Hartree Fock and Density Functional Theory (DFT)/B3LYP method using varied basis sets combination. The scaled B3LYP/6-311++G(d,p) results precisely complements with the experimental findings. Electronic absorption spectra along with energy and oscillator strength were obtained by TDDFT method. Atomic charges have also been reported. Total density isosurface and total density mapped with electrostatic potential surface (MESP) has been shown.

Introduction

Organic compounds add up to largest area of research. About half of the acknowledged organic compounds enclose at least one heterocyclic component. Ability to manifest substituents around a core scaffold in defined three dimensional representations is like a significant feature embraces by heterocyclic armamentarium. Emphasizing on this feature, heterocyclic compounds are exploited to great advantage by various researchers. These researches contribute in growth of society and improve the quality of life. Benzothiazole is one of the most promising sulphur and nitrogen containing aromatic heterocyclic scaffold, formed by the fusion between phenyl and thiazolyl rings. Its analogs incessantly attract the interest of chemists on account of their application to cure diseases like Alzheimer [1], cancer [2], rheumatic arthritis, diabetes [3], malaria [4,5], allergy, viral [6], and inflammation [7]. In

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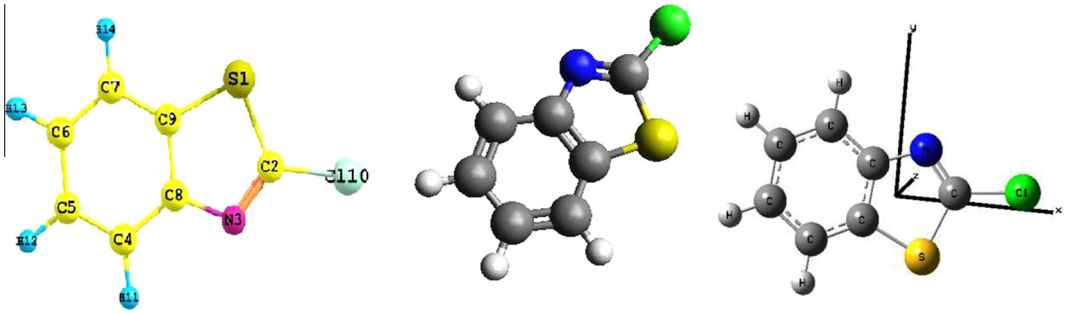

Fig. 1. Thermodynamically preferred geometry of 2-chlorobenzothiazole in accordance with atom numbering.

Table 1
Structural parameters of 2-chlorobenzothiazole obtained through HF and DFT method using varied basis sets.

Structural Parameters	HF/6-31G(d,p)	B3LYP/6-311++G(d,p)	B3LYP/6-31G(d,p)	HF/6-311++G(d,p)	Experimental[a]
Internuclear distance (Å)					
R(1,2)	1.75	1.76	1.77	1.74	1.732
R(1,9)	1.74	1.75	1.75	1.74	1.740
R(2,3)	1.25	1.27	1.28	1.25	1.353
R(2,10)	1.71	1.73	1.73	1.71	1.730
R(3,8)	1.39	1.38	1.39	1.39	1.380
R(4,5)	1.37	1.38	1.38	1.37	1.353
R(4,8)	1.39	1.39	1.40	1.37	1.391
R(4,11)	1.07	1.08	1.08	1.07	
R(5,6)	1.39	1.40	1.40	1.39	1.384
R(5,12)	1.07	1.08	1.08	1.07	
R(6,7)	1.37	1.39	1.39	1.37	1.395
R(6,13)	1.07	1.08	1.08	1.07	1.380
R(7,9)	1.38	1.39	1.39	1.38	1.380
R(7,14)	1.07	1.08	1.08	1.07	
R(8,9)	1.39	1.41	1.41	1.39	1.380
Bond angle (°)					
A(2,1,9)	87.57	87.61	87.54	87.61	92.3
A(1,2,10)	119.01	118.89	118.81	118.99	
A(3,2,10)	123.11	123.59	123.51	123.18	
A(5,4,8)	118.61	118.84	118.83	118.61	120.5
A(5,4,11)	121.80	121.77	121.88	121.69	
A(8,4,11)	119.58	119.37	119.27	119.68	
A(4,5,6)	120.89	120.95	120.93	120.90	118.6
A(4,5,12)	119.70	119.61	119.61	119.69	
A(6,5,12)	119.40	119.42	119.45	119.39	
A(5,6,7)	120.99	121.07	121.12	120.93	121.6
A(5,6,13)	119.54	119.61	119.59	119.57	
A(7,6,13)	119.45	119.31	119.28	119.48	
A(6,7,9)	117.93	117.92	117.93	117.93	120.6
A(6,7,14)	120.88	120.77	120.80	120.86	
A(9,7,14)	121.18	121.30	121.25	121.20	
A(3,8,4)	124.59	124.96	124.75	124.65	124.8
A(3,8,9)	115.29	115.36	115.54	115.25	112.0
A(4,8,9)	120.10	119.66	119.69	120.09	119.0
A(1,9,7)	129.50	129.30	129.34	129.47	
A(1,9,8)	109.03	109.16	109.18		110.0
A(7,9,8)	121.45	121.53	121.46	121.51	121.4
Dihedral angles (°)					
D(9,1,2,10)	180.0	180.0	180.0	180.0	180.0
D(2,1,9,7)	180.0	180.0	180.0	180.0	180.0
D(2,1,9,8)	0.0	0.0	0.0		0.0
D(10,2,3,8)	180.0	180.0	180.0	180.0	180.0
D(2,3,8,4)	180.0	180.0	180.0	180.0	180.0
D(2,3,8,9)	0.0	0.0	0.0	0.0	0.0
D(8,4,5,6)	0.0	0.0	0.0	0.0	0.0
D(8,4,5,12)	180.0	180.0	180.0	180.0	180.0
D(11,4,5,6)	180.0	180.0	180.0	180.0	180.0
D(11,4,5,12)	0.0	0.0	0.0	0.0	0.0
D(5,4,8,9)	0.0	0.0	0.0	0.0	0.0
D(11,4,8,3)	0.0	0.0	0.0	0.0	0.0
D(11,4,8,9)	180.0	180.0	180.0	180.0	180.0
D(4,5,6,7)	0.0	0.0	0.0		
D(4,5,6,13)	180.0	180.0	180.0	180.0	180.0
D(12,5,6,7)	180.0	180.0	180.0	180.0	180.0

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