Oriental Journal of Chemistry Vol. **26**(1), 251-254 (2010)

Theoretical study of the crystal structure of 4-chloro-N-(3-chlorophenyl)benzamide

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(Received: November 30, 2009; Accepted: January 10, 2010)

ABSTRACT

The geometrical parameters of 4-Chloro-N-(3-chlorophenyl)benzamide were calculated theoretically using Gaussian03 set of quantum chemistry codes. The obtained geometrical parameters are compared with the reported XRD structure of 4-Chloro-N-(3-chlorophenyl) benzamide. The bond lengths and bond angles calculated theoretically agree with the reported values.

Key words: 4-Chloro-N-(3-chlorophenyl)benzamide, HF calculations, XRD.

INTRODUCTION

enzamide derivatives exhibit various types of biological properties such as anthelmentic, antihistaminic, antifungal, and antibacterial[1-9]. Arslan *et al*.[10] reported the molecular structure and vibrational spectra of 2-chloro-N-(diethyl carbamothioyl) benzamide by Hartree-Fock and density functional methods. Takeuchi *et al*.[11] reported the molecular structure of benzamide as studied by gas phase electron diffraction. In the past few decades, the dramatically rising prevalence of multidrug-resistant microbial infections has become a serious health care problem. In particular, the emergence of multi-drug resistant strains of Gram-positive bacterial pathogens such as methicillin-resistant *Staphylococcus aureus* and *Staphylococcus epidermis* and vancomycin-resistant *Enterococcus* is a problem of ever-increasing significance[12-16]. Nayak *et al*.[17] reported the crystal structure of the title compound. In the present study, we have calculated the geometrical parameters of 4-Chloro-N-(3-chlorophenyl) benzamide theoretically and compared with the reported values

RESULTS AND DISCUSSION

The geometry of the title compound is optimized (Figure 1) by using Gaussian03 software[18]

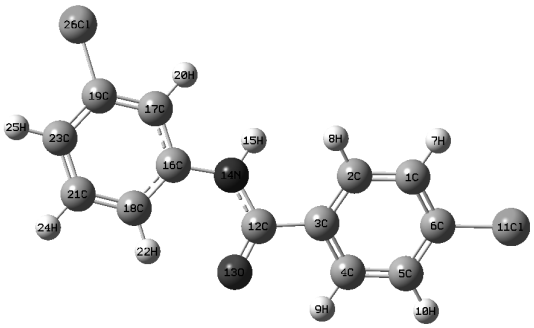

Fig. 1: Optimized geometry

at HF/3-21G* level. The optimized geometrical parameters are given in Table 1. For the benzamide moiety of the title compound, the HF calculations give the bond lengths C_3-C_{12}, C_{12}-O_{13}, C_{12}-N_{14}, N_{14}-H_{15}, N_{14}-C_{16} as 1.4969, 1.2195, 1.3641, 0.9964, 1.4089Å whereas the corresponding reported values are 1.4913, 1.2262, 1.3442, 0.8, 1.4123 Å, respectively[17]. The C=O and C-N bond lengths in benzamide, acetamide, formamide, are, respectively, 1.2253, 1.2203, 1.2123 Å and 1.3801, 1.3804, 1.3684 Å[19]. Kurt[20] reported the CCl bond length as 1.757 Å and Nayak *et al*.[17] reported the CCl bond lengths C_6-Cl_{11} =1.7382 Å, C_{19}-Cl_{26} =1.7402 Å. In the present study the CCl bond lengths are 1.7491 and 1.744 Å. The C-C bond lengths in the 1,4- and 1,3-substituted phenyl rings lie in the range 1.3723-1.3943 Å and 1.3694-1.3863 Å, respectively[17], whereas the calculated ranges are 1.3785-1.3858 Å and 1.3758-1.3907 Å. The C-C bond length of benzene[21] is 1.399 Å and of benzaldehyde[22] is 1.3973Å. The CH bond length is reported[17] as 0.93Å and the calculated values are in the ranges, 1.0967-1.0713 Å and 1.0639-1.0715 Å. The reported values of the bond angles[17], around C_{19} and C_6 positions are, C_{23}-C_{19}-Cl_{26} =119.3, C_{17}-C_{19}-Cl_{26} =118.5, C_{17}-C_{19}-C_{23} =121.4, C_1-C_6-Cl_{11} =119.4, C_5-C_6-Cl_{11} =119.4 and C_1-C_6-C_5 =120.7º and these values are in agreement with the calculated values (Table 1). For the title compound, the HF calculations give the bond angles C_{18}-C_{16}-N_{14}, C_{17}-C_{16}-N_{14}, C_{16}-N_{14}-H_{15}, C_{16}-N_{14}-C_{12}, N_{14}-C_{12}-O_{13}, N_{14}-C_{12}-C_3, H_{15}-N_{14}-C_{12}, O_{13}-C_{12}-C_3, C_{12}-C_3-C_2, C_{12}-C_3-C_4 as 123.7, 117.1, 114.8, 127.7, 123.7, 115.6, 117.3, 120.7, 124.1, 116.4º whereas the corresponding XRD values[17] are, 123.9, 116.5, 115.9, 128.2, 121.9, 117.1, 115.9, 120.9, 124.0, 118.4º, respectively. The values of the angles C_{12}-C_3-C_4 (116.4) and O_{13}-C_{12}-C_3 (120.7) are smaller than those of benzaldehyde[22] 121.0º and 123.6º. Nayak et al.[17] reported the dihedral angles C_{16}-N_{14}-C_{12}-O_{13} = 6.8, N_{14}-C_{12}-C_3-C_2 = 21.8, O_{13}-C_{12}-C_3-C_2 = -157.4, C_{21}-C_{23}-C_{19}-Cl_{26} = 179.3, C_{16}-C_{17}-C_{19}-Cl_{26} = -179.0, C_4-C_5-C_6-Cl_{11} = 179.1, C_2-C_1-C_6-Cl_{11} = 178.6º whereas the calculated values are 5.4, 22, -159.3, 180.0, -180.0, 179.9 and 179.7º, respectively.

Table 1: Optimized geometrical parameters

Bond lengths (Å)		Bond Angles (º)		Dihedral Angles (º)	
C_1-C_2	1.3822	A(2,1,6)	119.6	D(6,1,2,3)	-0.1
C_1-C_6	1.3799	A(2,1,7)	120.6	D(6,1,2,8)	177.8
C_1-H_7	1.0698	A(6,1,7)	120.0	D(7,1,2,3)	-179.5
C_2-C_3	1.3858	A(1,2,3)	120.4	D(7,1,2,8)	-1.7
C_2-H_8	1.0713	A(1,2,8)	118.5	D(2,1,6,5)	-0.8
C_3-C_4	1.3858	A(3,2,8)	121.1	D(2,1,6,11)	179.7
C_3-C_{12}	1.4969	A(2,3,4)	119.4	D(7,1,6,5)	178.6
C_4-C_5	1.3795	A(2,3,12)	124.1	D(7,1,6,11)	-0.9
C_4-H_9	1.0697	A(4,3,12)	116.4	D(1,2,3,4)	1.4
C_5-C_6	1.3808	A(3,4,5)	120.6	D(1,2,3,12)	179.1
C_5-H_{10}	1.0698	A(3,4,9)	118.7	D(8,2,3,4)	-176.4
C_5-Cl_{11}	1.7440	A(5,4,9)	120.8	D(8,2,3,12)	1.3
C_{12}-O_{13}	1.2195	A(4,5,6)	119.2	D(2,3,4,5)	-1.9
C_{12}-N_{14}	1.3641	A(4,5,10)	120.8	D(2,3,4,9)	178.0
O_{13}-H_{22}	2.1546	A(6,5,10)	120.0	D(12,3,4,5)	-179.7
N_{14}-H_{15}	0.9964	A(1,6,5)	121.0	D(12,3,4,9)	0.2
N_{14}-C_{16}	1.4089	A(1,6,11)	119.4	D(2,3,12,13)	-159.3
C_{16}-C_{17}	1.3907	A(5,6,11)	119.6	D(2,3,12,14)	22.0

Table 1. Cont...

C_{16}-C_{18}	1.3902	A(3,12,13)	120.7	D(4,3,12,13)	18.5
C_{17}-C_{19}	1.3758	A(3,12,14)	115.6	D(4,3,12,14)	-160.2
C_{17}-H_{20}	1.0711	A(13,12,14)	123.7	D(3,4,5,6)	1.0
C_{18}-C_{21}	1.3822	A(12,14,15)	117.3	D(3,4,5,10)	-179.3
C_{18}-H_{22}	1.0639	A(12,14,16)	127.7	D(9,4,5,6)	-178.9
C_{19}-C_{23}	1.3784	A(15,14,16)	114.8	D(9,4,5,10)	0.8
C_{19}-Cl_{26}	1.7491	A(14,16,17)	117.1	D(4,5,6,1)	0.4
C_{21}-C_{23}	1.3823	A(14,16,18)	123.7	D(4,5,6,11)	179.9
C_{21}-H_{24}	1.0715	A(17,16,18)	119.2	D(10,5,6,1)	-179.3
C_{23}-H_{25}	1.0695	A(16,17,19)	120.1	D(10,5,6,11)	0.2
		A(16,17,20)	120.5	D(3,12,14,15)	8.7
		A(19,17,20)	119.4	D(3,12,14,16)	-176.0
		A(16,18,21)	119.5	D(13,12,14,15)	-169.9
		A(16,18,22)	119.4	D(13,12,14,16)	5.4
		A(21,18,22)	121.1	D(12,14,16,17)	179.7
		A(17,19,23)	121.4	D(12,14,16,18)	-0.0
		A(17,19,26)	118.9	D(15,14,16,17)	-4.9
		A(23,19,26)	119.7	D(15,14,16,18)	175.4
		A(18,21,23)	121.6	D(14,16,17,19)	-179.7
		A(18,21,24)	119.0	D(14,16,17,20)	0.3
		A(23,21,24)	119.4	D(18,16,17,19)	0.1
		A(19,23,21)	118.2	D(18,16,17,20)	180.0
		A(19,23,25)	120.4	D(14,16,18,21)	179.5
		A(21,23,25)	121.4	D(14,16,18,22)	-0.9
				D(17,16,18,21)	-0.2
				D(17,16,18,22)	179.4
				D(16,17,19,23)	0.1
				D(16,17,19,26)	-180.0
				D(20,17,19,23)	-179.8
				D(20,17,19,26)	0.1
				D(16,18,21,23)	0.2
				D(16,18,21,24)	-180.0
				D(22,18,21,23)	-179.4
				D(22,18,21,24)	0.4
				D(17,19,23,21)	-0.1
				D(17,19,23,25)	180.0
				D(26,19,23,21)	180.0
				D(26,19,23,25)	0.0
				D(18,21,23,19)	-0.0
				D(18,21,23,25)	179.9
				D(24,21,23,19)	-179.9
				D(24,21,23,25)	0.1

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