IDENTIFICATION OF ELECTROPHILIC AND NUCLEOPHILIC CENTERS IN PHENYL-2-CHLOROPROPIONATE

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Abstract

In this study, the nucleophilic and electrophilic centers of the phenyl-2-chloropropionate molecule were identified and analyzed using atomic charge values calculated with the HyperChem software package (CNDO, INDO, MNDO, AM1, RM1, PM3 methods). The distribution of atomic charges enabled the determination of reactive sites within the molecule.

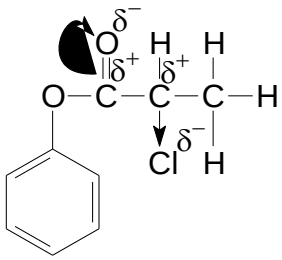
Keywords: phenyl-2-chloropropionate, HyperChem, nucleophilic, electrophilic, structure, charge, molecule, ester, carbonyl group, halogen, reaction, reaction center.

Introduction

Quantum chemical calculation methods play an important role in determining the electronic structure and reactivity of the synthesized phenyl-2-chloropropionate molecule. By studying the distribution of electron density within the molecule, it is possible to identify its nucleophilic and electrophilic centers. These centers indicate which parts of the molecule actively participate during chemical reactions [1,3]

Main Part

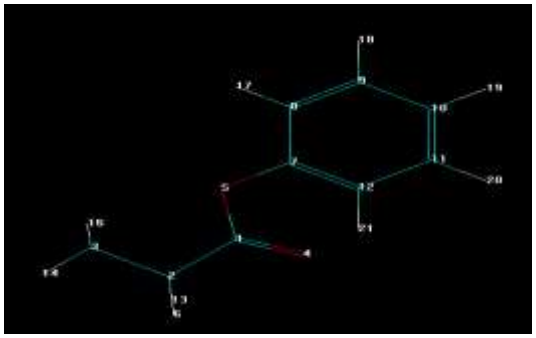
The studied molecule consists of an aromatic benzene ring and several functional groups, and its general structure can be represented as follows.



The molecule contains an ester bond (–O–), a carbonyl group (C=O), and a chlorine atom as a halogen substituent. These functional groups significantly influence the distribution of electron density within the molecule [2].

According to the calculation results, the main nucleophilic centers in the molecule are the oxygen atoms and the chlorine atom. The carbonyl oxygen is considered the strongest nucleophilic center in the molecule due to its high electronegativity and the presence of lone electron pairs. In addition, the oxygen atom in the ester bond participates in resonance interaction with the benzene ring, increasing electron density and exhibiting nucleophilic properties. The chlorine atom, being an electronegative element, also attracts electron density and carries a partial negative charge.

The numbering and three-dimensional structure of phenyl-2-chloropropionate are presented as follows.



To identify nucleophilic and electrophilic centers, atomic charge values were calculated using the HyperChem software package (CNDO, INDO, MNDO, AM1, RM1, PM3 methods), and the following data were obtained.

Table

Atomic charge values of phenyl-2-chloropropionate calculated using HyperChem (CNDO, INDO, MNDO, AM1, RM1, PM3 methods).

№	Atoms	Hyperchem					
		CNDO	**INDO**	**MNDO**	**AM1**	**RM1**	**PM3**
1	C_1	0,450	0.513	0.352	0.029	0.334	0.358
2	C_2	-0,034	0.250	0.093	-0.056	0.087	-0.072
3	C_3	0.026	0.058	0.025	-0.220	-0.152	-0.128
4	O_4	-0,337	-0.377	-0.328	-0.311	-0.317	-0.345
5	O_5	-0.331	-0.348	-0.268	-0.221	-0.232	-0.203
6	Cl_6	-0.060	-0,422	-0.0171	-0.075	-0.237	-0.022
7	C_7	0.401	0.445	0.091	0.057	0.058	0.068
8	C_8	-0,206	-0.191	-0.055	-0.129	-0.094	-0.106
9	C_9	0.109	0.117	-0.050	-0.119	-0.090	-0.088
10	C_{10}	-0.170	-0.117	-0.056	-0.134	-0.100	-0.104
11	C_{11}	-0.113	0.116	-0.049	-0.114	-0.085	-0.088

12	C_{12}	-0,223	-0.181	-0.052	-0.134	-0,092	-0.103
13	C_{13}	0.067	0.073	0.065	0.144	0.127	0.101
14	C_{14}	0.077	0.087	0.019	0.098	0.076	0.060
15	C_{15}	0,069	0.057	0.029	0.011	0.071	0.057
16	C_{16}	0.152	0.127	0.012	0.094	0.090	0.066
17	C_{17}	-0,029	-0.042	0.071	0.146	0.116	0.115
18	C_{18}	-0,041	-0.054	0.064	0.136	0.105	0.105
19	C_{19}	-0.024	-0.031	0.064	0.135	0.105	0.105
20	C_{20}	-0.041	-0.052	0.065	0.138	0.105	0.105
21	C_{21}	-0,038	-0.027	0.076	0.153	0.123	0.118

The table data show that the oxygen atoms (O_4 and O_5) in the molecule possess negative charge values across all semi-empirical methods. For example, the charge values for the O_4 atom are −0.337 (CNDO), −0.377 (INDO), −0.328 (MNDO), −0.311 (AM1), −0.317 (RM1), and −0.345 (PM3). Similarly, the O_5 atom also exhibits negative charges in all methods, with values ranging from −0.331 to −0.221. This behavior is explained by the high electronegativity of oxygen atoms. Oxygen atoms attract electron density, creating electron-rich regions within the molecule. Therefore, these atoms act as nucleophilic centers.

The chlorine atom (Cl_6) also shows significantly negative charge values in some methods. For instance, in the INDO method, its charge is −0.422, indicating a high electron density around the chlorine atom. Thus, the chlorine atom can also exhibit nucleophilic properties to a certain extent.

In contrast, some carbon atoms in the table exhibit partial positive charges. In particular, the charge values for the C_1 atom are 0.450 (CNDO), 0.513 (INDO), 0.352 (MNDO), 0.334 (RM1), and 0.358 (PM3), indicating that this atom is one of the most

positively charged centers in the molecule. This carbon atom belongs to the carbonyl group, and due to the strong electron-withdrawing effect of the oxygen atom, an electron deficiency arises at this site. Therefore, the C_1 atom is considered the primary electrophilic center in the molecule.

Additionally, the C_7 atom also shows positive charge values across all methods (0.401; 0.445; 0.091; 0.057; 0.058; 0.068), making it another electrophilic center. The C_3 atom, however, exhibits positive charge values in some methods (CNDO and INDO), while negative values are observed in AM1, RM1, and PM3 methods. This indicates that the electron density at this atom is intermediate.

Overall, the table results indicate that electron density in the molecule is mainly concentrated on the oxygen atoms and partially on the chlorine atom. Therefore, these atoms serve as nucleophilic reactive centers. In contrast, electron deficiency is observed at the carbonyl carbon and some other carbon atoms, which act as electrophilic centers.

Conclusion

Thus, in the phenyl-2-chloropropionate molecule, the main nucleophilic centers are identified as O_4, O_5, and partially Cl_6 atoms, while the primary electrophilic centers are C_1 and C_7 atoms. These results are important for explaining the chemical behavior and reactivity of the molecule in chemical reactions.

The calculation results indicate that the carbon atom in the carbonyl group is the strongest electrophilic center in the molecule. This is due to the high electronegativity of the oxygen atom, which withdraws electron density from the carbonyl carbon. As a result, a partial positive charge is formed on the carbonyl carbon, making it the primary site for nucleophilic attack.

Furthermore, the carbon atom bonded to the chlorine atom also exhibits electrophilic properties, since chlorine, being an electronegative atom, attracts electron density toward itself.

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