УДК 538.9
doi: 10.18101/ 978-5-9793-0898-2-97-103

SOME RESULTS OF CINNAMOYL CHLORIDE (C_9H_7CLO) ORGANIC CRYSTAL

© ***Otgontuul J.***, Institute of Physics and Technology,
Mongolian Academy of Science
Ulaanbaatar, Mongolia
E-mail: tuul345@yahoo.com

© ***Sevjidsuren G.***, Institute of Physics and Technology,
Mongolian Academy of Science
Ulaanbaatar, Mongolia

© ***Altantsog P.***, Institute of Physics and Technology,
Mongolian Academy of Science
Ulaanbaatar, Mongolia

Single crystals of the β-form of CACI were grown from oversaturated hexane solutions by slow cooling from 50°C to room temperature. The molecular and crystal structures of cinnamoyl chloride were determined using (HKL) file, which shows the results of experimental STOE STADI 4 four-circle diffractometer. The bandwidth and density of states for cinnamoyl chloride (C_9H_7CLO) were calculated using "CRYSTAL" program.
Keywords: cinnamoyl chloride, bandwidth, conductor, light-induced, crystal structure

Introduction

The organic components play major role on the research of modern new materials, due to their physical and chemical features. One of them is cinnamoyl chloride (C_9H_7CLO) and its structural variation mechanism and dynamics are being studied recently.Cinnamoyl chloride (C_9H_7CLO) is much induced to light it is a common system suitable for researching the mechanism of phase variations, which are held in crystal by light influence and the phenomenon, which is held by light influence are much used at the technique in recent time.

For example, it is possible to be used for transferring information and making organic diode conductor for the electronics. However, the phase variations of light-induced organic crystals have been determined since

1960, but its mechanism of structural variation caused light interaction has not been clearly understood [1].

I. Experiment

Cinnamoyl chloride (C_9H_7CLO) organic crystals were grown from oversaturated hexane solutions by slow cooling from 50°C to room temperature. The crystal and molecular structure of cinnamoyl chloride (C_9H_7CLO) was determined by using "SHELXTL" package program and by collecting the diffraction data from STOE STADI 4 four-circle diffractometer.

In order to measure the sample at the diffractometer STOE STADI 4 for monocrystals, the sample has to be fixed on the goniometer head using the amorph stick and glue Plus 5 are used. The glue was little pasted to the amorph stick and chosen crystal was pasted to the amorph stick on the goniometer head. The measurement was performed at 293^0K by 7 hours using STOE STADI 4 four-circle diffractometer with in $\omega/2\theta$ scan mode with niobium monochromated Mo K_α radiation.

II. Results and Discussion

Experiment results:

The crystal and molecule structures of cinnamoyl chloride (C_9H_7CLO) were determined by using "SHELXTL" package program and by collecting the diffraction data from STOE STADI 4 four-circle diffractometer.

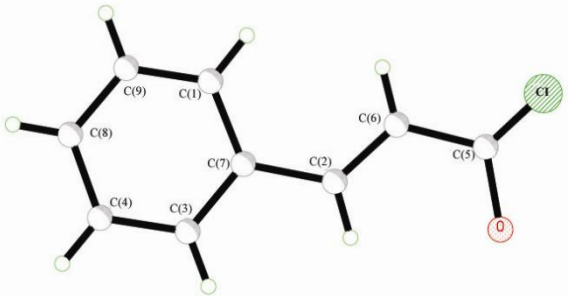

Fig. 1. Molecule structure of cinnamoyl chloride using SHELXTL program from experimental method

The unit cell of crystal lattice for cinnamoyl chloride (C_9H_7CLO) was determined by (HKL) file, which are the results of diffractometer

measurement for homogeneous single crystal and using the SHELXTL package program.

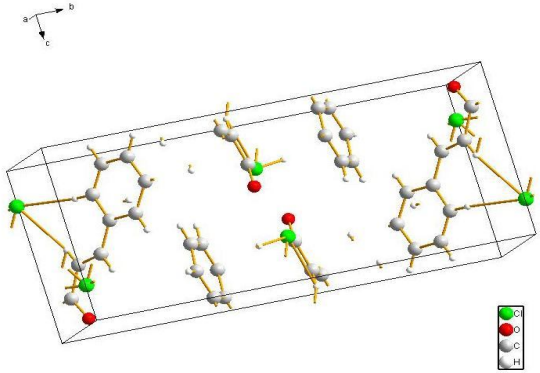

Fig. 2. The unit cell of cinnamoyl chloride (C_9H_7CLO) from experimental data

Table 1

Data of crystal structure for cinnamoyl chloride (C_9H_7CLO)

Crystal system :	Monoclinic
Space group :	P2(1)/n
Unit cell :a	5.520 Å
Unit cell: b	17.51 Å
Unit cell : c	7.700 Å
Unit cell :α	90.000^0
Unit cell :β	96.770^0
Unit cell :γ	90.000^0
Volume : V	$450.0Å^3$
Z	4

The charge density of cinnamoyl chloride (C_9H_7CLO) was estimated on the plane [110] using the SHELXTL program and it gives information of chemical bond. Therefore along line from C9 to O covalent bonding is dominated; along line from C1 to C9 and from C9 to CL, the atoms are bounded by ion bonding.

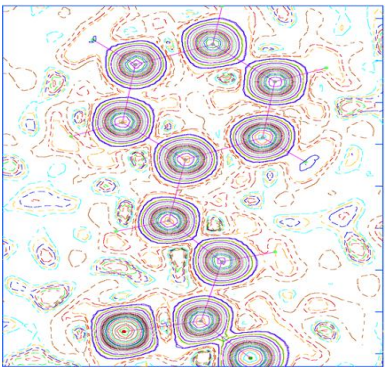

Fig. 3. Charge density of cinnamoyl chloride (C_9H_7CLO) was determined by using the "SHELXTL" program

Interatomic distancesand interatomic angles of cinnamoyl chloride (C9H7CLO) were determined by using "SHELXTL" package program and by collecting the diffraction data from STOE STADI 4 four-circle diffractometer.

Table2

Interatomic distancesand interatomic angles from the experiment

Interatomic distances, Å			
O-C5	1.336	C1-C9	1.355
C1-C7	1.412	C2-C6	1.332
C3-C7	1.387	C4-C8	1.398
C5-C6	1.461	C1-C5	1.398
C3-C4	1.404	C2-C7	1.483
Interatomic angles, ^{0}			
C1-C5-C6	122.3	O-CL-C5	122.8
C6-C2-C7	126.4	C4-C3-C7	120.7
C1-C7-C2	122.8	C3-C7-C1	118.5
O-C5-C6	122.3	C4-C8-C9	119.7
C8-C4-C3	119.1	C1-C9-C8	121.4

Theoretical results

The bandwidth, density of states, Fermi energy and data of the crystal structure were calculated using CRYSTAL program. The CRYSTAL package performs ab-initio calculations of the ground state energy , elec-

tronic wave function and properties of periodic systems. Near bandwidth calculation of Fermi level is very attractive. In order to make estimation the crystal geometric, symmetric data, basic variability and mathematical details of the atoms for cinnamoyl chloride (C_9H_7CLO) were prepared into the input file.

From the bandwidth calculation the cinnamoyl chloride has 624 energy bands, which contains 120 energy bands for core electron and 324 energy bands for valence electron. The band gap was estimated from 0.07 to 0.1eV, which means cinnamoyl chloride is conductor. Also, we have calculated density of states, which shows that probability of electron concentration the band. Figure 4 shows the theoretical result density of states and bandwidth of cinnamoyl chloride (C_9H_7CLO).

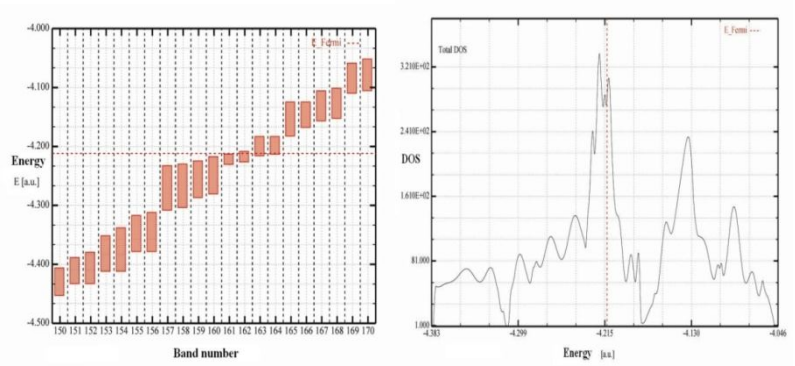

Fig. 4.The bandwidth, density of states, Fermi energy and data of the crystal structure were calculated using CRYSTAL program

From the results of density of states, Fermi energy was estimated by E_F=-4.215[a.u]. Interatomic distances and interatomic angles were defined in accordance with theoretical calculation. Table 3 shows the theoretical result interatomic distanceand interatomic angle of cinnamoyl chloride (C_9H_7CLO).

Table 3

Interatomic distances and interatomic anglesfrom the theoretical results

Interatomic distances, Å			
O-C5	1.337	C1-C9	1.357
C1-C7	1.387	C2-C6	1.330
C2-C7	1.486	C3-C7	1.398
C3-C4	1.403	C1-C5	1.479
C5-C6	1.459	C4-C8	1.385
Interatomic angles^0			
C9-C1-C7	119.6	C6-C2-C7	126.3
C4-C3-C7	120.6	C8-C4-C3	119.0
CL-C5-O	121.9	CL-C5-C6	121.3
O-C5-C6	121.8	C2-C6-C5	123.3
C3-C7-C1	118.6	C1-C7-C2	122.6
C4-C8-C9	119.8	C1-C9-C8	121.3

IV. Conclusion

Cinnamoyl chloride (C_9H_7CLO) organic crystals were grown from oversaturated hexane solutions by slow cooling from 50°C to room temperature.

The unit cell of cinnamoyl chloride (C_9H_7CLO) is consisted with 4 molecules and its crystal system has the following parameters:a = 5.520Å, b=17.51Å, c=7.700Å, $\alpha=90.000^0$, $\beta=96.770^0$, $\gamma=90.00^0$,volume V=450Å^3. The bandwidth, density of states, Fermi energy and data of the crystal structure were calculated using CRYSTAL program. From the bandwidth calculation cinnamoyl chloride (C_9H_7CLO) has 624 energy bands, which contains 120 energy bands for core electron and 324 energy bands for valence electron.From the results of density of states, Fermi energy was estimated by E_F = -4.215 [a.u].The band gap was estimated from 0.07 to 0.1eV, which means cinnamoyl chloride is conductor.

By using the "SHELTXL" program, the interatomic distances was defined as 1.33-4.47Å , by using the "CRYSTAL" program, the interatomic distances was defined as 1.33-4.49Å . Interatomic angles, which were determined with "SHELTXL" program, were defined as $118.5\text{-}126.4^0$ and interatomic angles, determined with "CRYSTAL" program, were defined as $118.6\text{-}126.3^0$. The research shows that the results of experiment and theoretical calculations are well suited.

Bibliography

1. Otgontuul J., Tserenchimed M., Altantsog P. ICMS, (2010) p92.
2. Davaasambuu J., Techert S., Phys J. D: Appl. Physics, (2005), 38, A204.
3. Davaasambuu J., Busse G., Techert S., Phys J. Chem. A110,(2006), 3261
4. Nakanishi H., Jones W., Thomas J.M., Chem J.C.S. Comm., (1980), 13, 611
5. Gohen M. D., Schmidt G.M.J., Chem J. Soc., (1964). 1996.
6. Chorev M., Goodman M. Trens Biotechnol. (1995), 13(10). 438.
7. Chan G.K.L. and Hardy N.C., Phys.Rev. A59, (1999) 3075.

РЕЗУЛЬТАТЫ ИССЛЕДОВАНИЯ
КРИСТАЛЛИЧЕСКОЙ СТРУКТУРЫ ЦИННАМОИЛХЛОРИДА

*Ж. Отгонтуул,*Институт физики и технологии
Монгольской Академии наук
Монголия, Улаанбаатар
E-mail: tuul345@yahoo.com

Г. Сэвжидсурэн, Институт физики и технологии
Монгольской Академии наук
Монголия, Улаанбаатар

П. Алтанцог, Институт физики и технологии
Монгольской Академии наук
Монголия, Улаанбаатар

Монокристаллы циннамоилхлорида (C_9H_7CLO) в β-форме были выращены из перенасыщенного раствора гексана при медленном охлаждении от50°С до комнатной температуры. Молекулярные и кристаллические структуры циннамоилхлорида были определены используя базу данных (HKL), котораясоздана из экспериментальных результатов, полученных на четырех цикловом дифрактометреSTOESTADI 4. Пропускная способность и плотность состояния для циннамоилхлорида (C_9H_7CLO) были рассчитаны с использованием программы "CRYSTAL".

Ключевые слова: циннамоил хлорид, полоса пропускания, проводник, кристаллическая структура.