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# Synthesis, Characterization, Spectroscopy of Tree new Aluminate (III) Complexes $[AlCl_3X](X= NO^-_3, CH_3COO^-, N^-_3)$ and Study of Antimicrobial Activities

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**Abstract:** The synthesis and characterization is reported of Tri new aluminate (III) complexes with general formula $Na[AlCl_3\ X]$, These compounds derived from alumina trichloride and related salts. Sodium Trichloronitratoaluminate, SCNA, Sodium Trichloroacetatoaluminate, SCAA, Sodium Trichloroazidoaluminate, SCAZA produced tri ionic aluminate complexes. They easily synthesized in a nearly quantitative yield by using direct reaction of $AlCl_3$ and KX. These compounds were characterized by IR, UV/Visible and Mass techniques. In this paper, the optimized geometries and frequencies of the stationary point and the minimum-energy paths are calculated at the B3LYP/B3LYP level of theory too. Theoretical calculation has been used for extraction of structural and spectroscopic data of these new synthesized complexes. The antibacterial activities of synthesized compounds were studied against the *Staphylococcus aureus*, *Escherichia coli*, *Staphylococcus Epidermidis, Estreptococo B and Shigella*.

**Key words:** Synthesis · Characterization · Aluminate compounds · Theoretical calculation · SCNA · SCAA · SCAZA · Antibacterial

## INTRODUCTION

In this investigation, we report on the synthesis, spectroscopic characterization and antimicrobial activity of Aluminate (III) complexes with trichloro ligands: $Na^+[AlCl_3(NO_3)]^-$, $Na^+[AlCl_3(CH_3COO)]^-$, $Na^+[AlCl_3(N_3)]^-$. Although the synthesis of the TrichloroX has been reported earlier, no research has been done so far on the Aluminate complexes of these ligands. Al (III) can form stable herami complexes with tetra coordinating atoms, 3Cl, X ($NO_3$, $CH_3COO$, $N_3$) atoms can be coordinated to the (AL) ion. Thus, the geometry of the molecule is a distorted herami with the 3Cl, X ($NO_3$, $CH_3COO$, $N_3$) symmetry group. Ligands $NO_3^-$, $CH_3COO^-$, $N_3^-$ in the basis state to belong to point group $D_3h$, $D_3h$, $D_8h$ respectively. The Al(1)–Cl(3) bond distance in the $Na^+[AlCl_3(NO_3)]^-$, $Na^+[AlCl_3\ (CH_3COO)]^-$, $Na^+[AlCl_3(N_3)]^-$, complexes respectively is 2.2367Å, 2.2485 Å, 2.2507 Å and also bond angle in the mentioned complexes respectively is Cl(3)-Al(1)-Cl(4) 112.8263, 111.145, 109.4175.

However, a recent report indicated that several ionic liquids have been applied in separation of various mixtures [1, 2]. Moreover, ionic liquid properties such as heat capacities and refractive index [3], luminescence properties [4], osmotic coefficients [5], enthalpy, density, heat capacity [6] and thermo physical properties [7] have been studies since their first synthesis. Therewith, following our previous studies about ionic liquids chemistry [8-10], we decide to improve our knowledge about these compounds by synthesis, characterisation and theoretical study of some new Aluminium-based ionic liquids. The antibacterial activities of synthesized compounds were studied against the *Staphylococcus aureus*, *Escherichia coli, Staphylococcus Epidermidis, Streptococcus B and Shigella*.

**Experimental:** All chemicals and reagents used for the syntheses were commercial products (Merck) and used without further purification. Solvents used for reactions were purified and dried by standard procedures.

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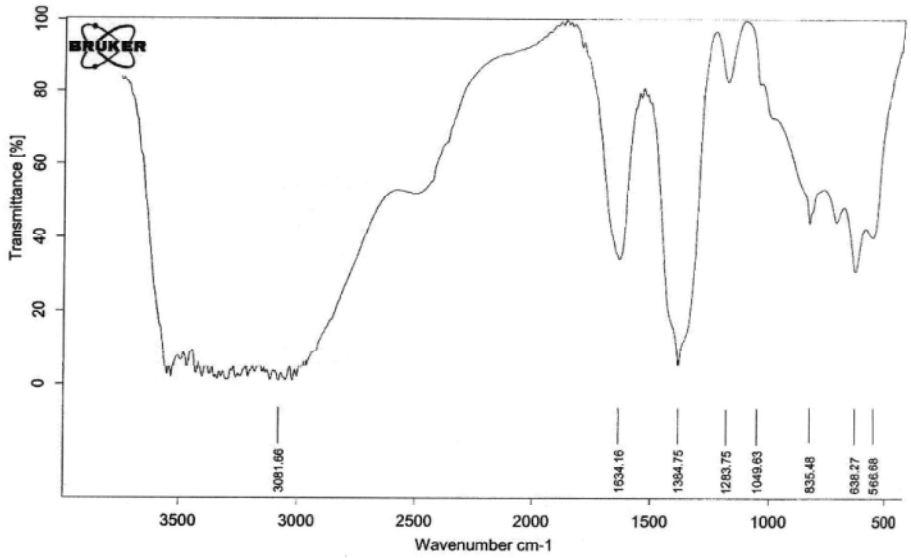


Fig. 1: The FT-IR spectrum of $Na^+[AlCl_3(NO_3)]^-$ (KBr Disk)

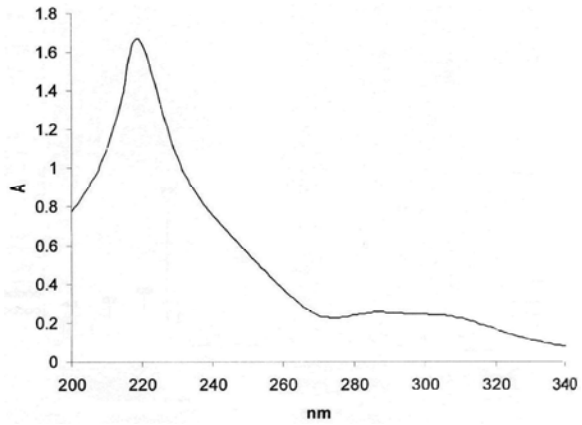


Fig. 2: The UV/Vis spectrum of $Na^+[AlCl_3(NO_3)]^-$

The molar conductance values of the complexes were measured in acetonitrile solution in room temperature with a Jenway 4510 conductometer instrument. Melting points were ascertained using an electrothermal apparatus and are uncorrected. The electronic spectroscopic data in 200–900 nm range were recorded in acetonitrile on a Perkin-Elmer lambda spectrophotometer. Infrared spectra were recorded as KBr disks on a Bruker Tensor model 420 spectrophotometer. Mass spectra were recorded on an Agilent Technology (HP) model Network Mass Selective Detector 5973 spectrophotometer.

**Sodium Trichloronitratoaluminate (III), $Na^+[AlCl_3(NO_3)]^-$:** Sodium trichloronitratoaluminate (III), $Na^+[AlCl_3(NO_3)]$ was prepared by dissolving $AlCl_3$ (0.3g, 2.3 mmol) in acetonitrile and adding this solution to a solution of $NaNO_3$ (0.195 g, 2.3 mmol) in acetonitrile under stirring at room temperature until a white precipitate was formed. After 3 hours stirring, the mixture was filtered, washed with ether and hexane. Precipitate amount was 0.46 gr; reaction randeman efficiency was 92%. MP: 280°C. *m/e* (%): 218 ($M^+$), 204, 180, 167, 157, 149, 125, 104, 89, 85, 73, 69, 57, 43; IR (KBr): 1384, 1283, 1049, 835, 638, 566 $cm^{-1}$ (Figure 1, 2).

**Sodium Trichloroacetatoaluminate (III), $Na^+[AlCl_3(CH_3COO)]^-$:** Sodium Trichloroacetatoaluminate (III), $Na^+[AlCl_3(CH_3COO)]^-$ was prepared by dissolving $AlCl_3$ (0.25g, 1.88 mmol) in acetonitrile and adding this solution to a solution of $NaCH_3COO$ (0.25 g, 1.84 mmol) in acetonitrile under stirring at room temperature until a white precipitate was formed. After 3 hours stirring, the mixture was filtered, washed with ether and hexane. Precipitate amount was 0.44gr. MP: 280°C. *m/e* (%): 215($M^+$), 180, 165, 152, 137, 97, 70, 43; IR (KBr): 1578, 1473, 1354, 1098, 1045, 702, 642, 522, 499, 420 $cm^{-1}$ (Figure 3, 4).

**Sodium Trichloroazidoaluminate (III), $Na^+[AlCl_3(N_3)]^-$:** Sodium trichloroazidoaluminate (III), $Na^+[AlCl_3(N_3)]$ was prepared by dissolving $AlCl_3$ (0.34g, 2.6 mmol) in acetonitrile and adding this solution to a solution of $NaN_3$ (0.16 g, 2.5 mmol) in acetonitrile under stirring at room temperature until a white precipitate was formed. After 3 hours stirring, the mixture was filtered, washed with ether and hexane. Precipitate amount was 0.45 gr. MP: 280°C. *m/e* (%): 199($M^+$), 104, 90, 76, 69, 50; IR (KBr): 2041, 1465, 639, 529, 471 $cm^{-1}$ (Figure 5, 6).

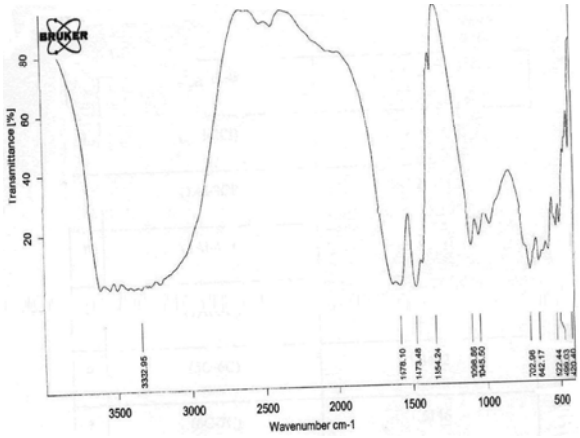


Fig. 3: The FT-IR spectrum of $Na^+[AlCl_3(CH_3COO)]^-$ (KBr Disk)

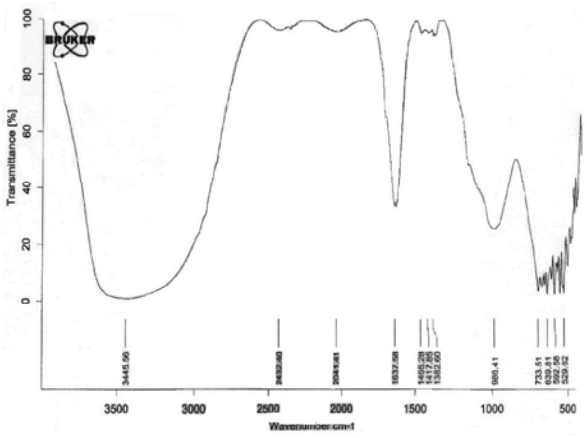


Fig. 5: The FT-IR spectrum of $Na^+[AlCl_3(N_3)]^-$ (KBr Disk)

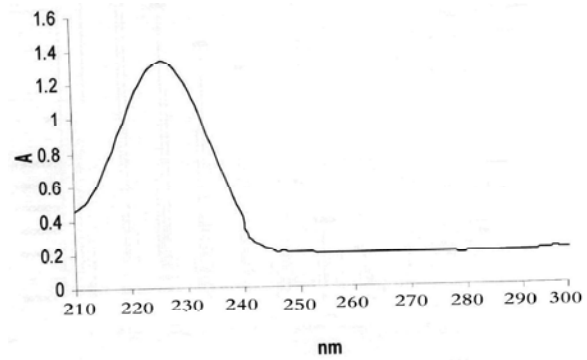


Fig. 4: The UV/Vis spectrum of $Na^+[AlCl_3(CH_3COO)]^-$

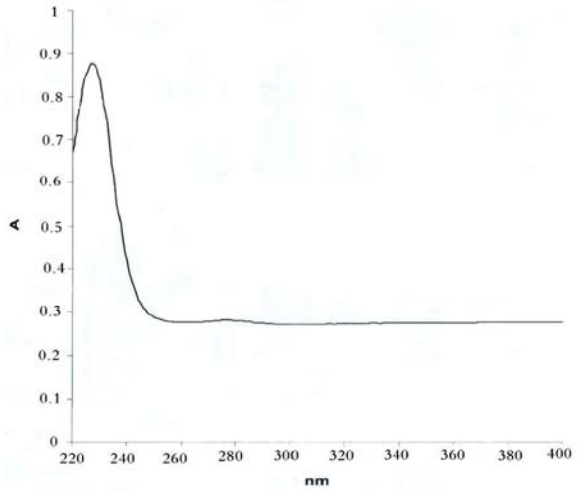


Fig. 6: The UV/Vis spectrum of $Na^+[AlCl_3(N_3)]^-$

**Computational Methods:** Density functional theory (DFT) calculations were carried out at B3LYP/LANL2DZ levels of theory with the Gaussian 98 package of programs [11, 12] which combines the exact Hartree-Fock exchange with Becke's and uses the Lee-Yang-Parr correlation function in order to include the most important correlation effects. The optimized structural parameters were used in the vibrational frequency calculations at the HF and DFT levels to characterize all stationary points as minima [13]. Harmonic vibrational frequencies (ν) in $cm^{-1}$ and infrared intensities (int) in Kilometer per mole of all compounds were performed at the same level on the respective fully optimized geometries.

**Antibacterial Activity Tests:** The *in vitro* activity tests were carried out using the Growth Inhibitory zone (well method), against the *Staphylococcus aureus*, *Escherichia coli*, *Staphylococcus Epidermidis, Streptococcus B and Shigella*. Microorganisms (obtained from enrichment cultures of the microorganisms in 1 mL Muller–Hinton broth, incubated at 37°C for 24 h) were cultured on Muller–Hinton agar medium. The inhibitory activities were compared with those of the standard medium using a 6 mm cork borer, 100 lL of solutions of the test compounds were poured into each well. The plates were incubated at 37°C overnight. The diameter of the inhibition zone was measured to the nearest millimeter. Each test was carried out in triplicate and the average was calculated for inhibition zone diameters. A blank containing only methanol showed no inhibition in a preliminary test. The macro-dilution broth susceptibility assay was used for the evaluation of minimal inhibitory concentration (MIC). Twelve test tubes was used for the macro-dilution method. By including 1 mL Muller–Hinton broth in each test and then adding 1 mL extract with concentration 100 mg/mL in the first tube, we made serial dilutions of this extract from first tube to last tube. Bacterial suspensions were prepared to match the turbidity of 0.5 McFarland turbidity standards. Matching this turbidity provides a bacterial inoculum concentration of 1.5×108 cfu/mL. Then 1 mL of bacterial suspension was added to each test tube. After incubation at 37°C for 24 h,

Table 1: *in vitro* antibacterial studies of the synthesized Compound.

| Compound | *Staphylococcus aureus* | *Staphylococcus Epidermidis* | *Streptococcus B* | *Escherichia coli* | *Shigella* |
|---|---|---|---|---|---|
| $Na[AlCl_3(NO_3)]$ | 3mm | - | - | 3mm | 3mm |
| $Na[AlCl_3(CH_3COO)]$ | 5mm | - | - | - | - |
| $Na[AlCl_3(N_3)]$ | 7mm | 8mm | - | - | 6mm |

the last tube in the series without turbidity was determined as the minimal inhibitory concentration (MIC) (Table 1).

## RESULTS AND DISCUSSION

$[AlCl_3X]^-$ can be prepared by the reaction of NaX and $AlCl_3$ derivative in dry acetonitrile. The complexes were found to be unsoluble in toluene and display good stability in air at room temperature. The structures of the ligands were confirmed by IR, UV and Mass data. The spectroscopic data of the $Na[AlCl_3$ X] complex and its complex show tri bands at (566, 1283), 702, 529 $cm^{-1}$ and these can be attributed to $X(NO_3$, $CH_3COO$, $N_3$ respectively). The comparison of experimental and accounting IR spectra's shown wich these two spectra have convergence relatively well together (Table 2-4). The electronic spectra of the complexes were measured in acetonitrile solution. The tri aluminate (III) complexes that were tested have moderate activity (inhibitory zones [15 mm) against all four positive gram bacteria, except Na $[AlCl_3X]$ that has weak activity toward S. aureus. Also indicate that the all tri complexes are moderately active against the two negative gram bacteria (inhibitory zones (15 mm), except for $AlCl_3X$ which shows weak activity toward pneumoniae.

Table 2: The comparison of experimental IR spectra results with accounting IR spectra results for composition SCNA

| Accounting | Experimental | Vibration species |
|---|---|---|
| 566 | 473 | Al-O |
| 493 | 638 | Al-Cl |

Table 3: The comparison of experimental IR spectra results with accounting IR spectra results for composition SCAA

| Accounting | Experimental | Vibration species |
|---|---|---|
| 466 | 420 | Al-Cl |
| 481 | 499 | Al-Cl |
| 617 | 702 | Al-O |

Table 4: The comparison of experimental IR spectra results with accounting IR spectra results for composition SCAZA

| Accounting | Experimental | Vibration species |
|---|---|---|
| 546 | 529 | Al-N |

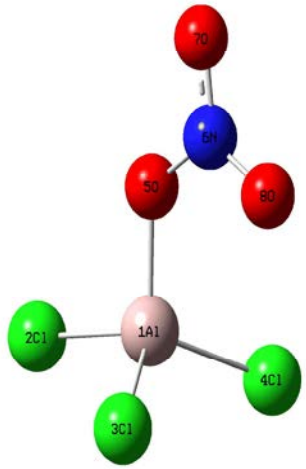


Fig. 7: Optimized molecular structures of $Na^+[AlCl_3(NO_3)]^-$ complex.

**Sodium Trichloronitratoaluminate (III), $Na^+[AlCl_3(NO_3)]^-$:** $Na^+[AlCl_3(NO_3)]^-$ was prepared by the reaction of $AlCl_3$ and $NaNO_3$ in acetonitrile solvent as follows:

$$NaNO_3 + AlCl_3 \rightarrow Na\,[AlCl_3(NO_3)]$$

In the vibrational spectrum of this compound, the known bands of cation and anion were seen such as $\nu_{Al\text{-}O\text{-}N}$ that was found at 566, 1283 $cm^{-1}$ and confirmed with literature data. In the mass spectra Na $[AlCl_3$ $(NO_3)]$ complex molecular weight peak related to m/e= 218 has been observed.

Figure 7. Optimized molecular structures of $Na^+[AlCl_3(NO_3)]^-$ complex: From the optimized structure of the title compounds, molecular parameters can be extracted. Molecular parameters can depict a useful representation of molecular structure. Therefore, we extracted important bond lengths and bond angles of computed complex and listed them in (Table 5-a, 5-b).

**Sodium Trichloroacetatoaluminate (III), $Na^+[AlCl_3$ $(CH_3COO)]^-$:** $Na^+[AlCl_3(CH_3COO)]^-$ was prepared by the reaction of $AlCl_3$ and $NaCH_3COO$ in acetonitrile solvent as follows:

$$NaCH_3COO + AlCl_3 \rightarrow Na\,[AlCl_3\,(CH_3COO)]$$

Table 5-a: Bond lengths [Å] for composition $Na^+[AlCl_3(NO_3)]^-$

| | Bond lengths | [Å] |
|---|---|---|
| 1 | Al(1)-Cl(2) | 2.2399 |
| 2 | Al(1)-Cl(3) | 2.2367 |
| 3 | Al(1)-Cl(4) | 2.237 |
| 4 | Al(1)-O(5) | 1.8615 |
| 5 | Al(1)-O(8) | 3.0116 |
| 6 | O(5)-N(6) | 1.3819 |
| 7 | N(6)-O(7) | 1.2483 |
| 8 | N(6)-O(8) | 1.2612 |

Table 5-b: Bond angles [°] for composition $Na^+[AlCl_3(NO_3)]^-$

| | Bond angles | [°] |
|---|---|---|
| 1 | Cl(2) Al(1)-Cl(3) | 110.0965 |
| 2 | Cl(2) Al(1)-Cl(4) | 110.0522 |
| 3 | Cl(2) Al(1)-O(5) | 100.7906 |
| 4 | Cl(3) Al(1)-Cl(4) | 112.8263 |
| 5 | Cl(3) Al(1)-O(5) | 111.2329 |
| 6 | Cl(3) Al(1)-O(8) | 85.5864 |
| 7 | Cl(4) Al(1)-O(5) | 111.2019 |
| 8 | Al(1)-O(5)-N(6) | 122.9855 |
| 9 | O(5)-N(6)-O(7) | 116.2822 |
| 10 | O(5)-N(6)-O(8) | 117. 5541 |
| 11 | O(7)-N(6)-O(8) | 126.1637 |
| 12 | Al(1)-O(8)-N(6) | 70.9102 |

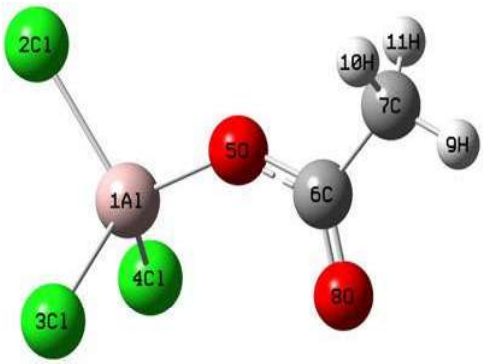


Fig. 8: Optimized molecular structures of $Na^+[AlCl_3(CH_3COO)]^-$ complex.

In the vibrational spectrum of this compound, the known bands of cation and anion were seen such as $\nu_{Al\text{-}O}$ that was found at 702cm$^{-1}$ and confirmed with literature data. In the Mass spectra Na $[AlCl_3(CH_3COO)]$ complex peak related to m/e=215.5 has been observed.

Figure 8. Optimized molecular structures of $Na^+[AlCl_3(CH_3COO)]^-$ complex: From the optimized structure of the title compounds, molecular parameters can be extracted. Molecular parameters can depict a useful representation of molecular structure. Therefore, we extracted important bond lengths and bond angles of computed complex and listed them in (Table 6-a, 6-b).

Table 6-a: Bond lengths [Å] for composition $Na^+[AlCl_3(CH_3COO)]^-$

| | Bond lengths | [Å] |
|---|---|---|
| 1 | Al(1)-Cl(2) | 2.2531 |
| 2 | Al(1)-Cl(3) | 2.2485 |
| 3 | Al(1)-Cl(4) | 2.2485 |
| 4 | Al(1)-O(5) | 1.7941 |
| 5 | O(5)-C(6) | 1.3442 |
| 6 | C(6)-C(7) | 1.5146 |
| 7 | C(6)-O(8) | 1.241 |
| 8 | C(7)-H(9) | 1.0913 |
| 9 | C(7)-H(10) | 1.0952 |
| 10 | C(7)-H(11) | 1.0952 |

Table 6-b: Bond angles [°] for composition $Na^+[AlCl_3(CH_3COO)]^-$

| | Bond angles | [°] |
|---|---|---|
| 1 | Cl(2) Al(1)-Cl(3) | 108.8671 |
| 2 | Cl(2) Al(1)-Cl(4) | 108.868 |
| 3 | Cl(2) Al(1)-O(5) | 104.6356 |
| 4 | Cl(3) Al(1)-Cl(4) | 111. 145 |
| 5 | Cl(3) Al(1)-O(5) | 111. 5321 |
| 6 | Cl(4) Al(1)-O(5) | 111.5279 |
| 7 | Al(1)-O(5)-C(6) | 137.5027 |
| 8 | O(5)-C(6)-C(7) | 112.4235 |
| 9 | O(5)-C(6)-O(8) | 124.4139 |
| 10 | C(7)-C(6)-O(8) | 123.1626 |
| 11 | C(6)-C(7)-H(9) | 110.0802 |
| 12 | C(6)-C(7)-H(10) | 109.6941 |
| 13 | C(6)-C(7)-H(11) | 109.6928 |
| 14 | H(9) -C(7)-H(10) | 110.0624 |
| 15 | H(9) -C(7)-H(11) | 110.059 |
| 16 | H(10) -C(7)-H(11) | 107.2057 |

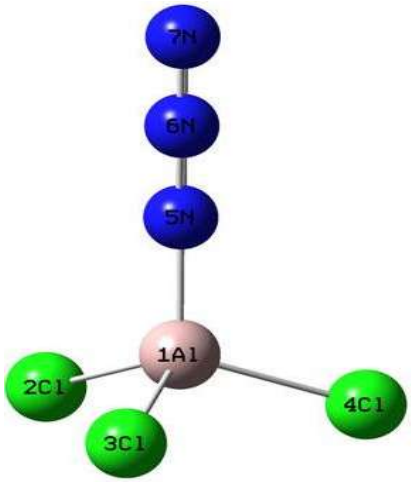


Fig. 9: Optimized molecular structures of Na $[AlCl_3(N_3)]$ complex.

**Sodium Trichloroazidoaluminate (III), $Na^+[AlCl_3(N_3)]^-$:** $Na^+[AlCl_3(N_3)]^-$ was prepared by the reaction of $AlCl_3$ and $NaN_3$ in acetonitrile solvent as follows:

Table 7-a: Bond lengths [Å] for composition $Na^+[AlCl_3(N_3)]^-$

| | Bond lengths | [Å] |
|---|---|---|
| 1 | Al(1)-Cl(2) | 2.2511 |
| 2 | Al(1)-Cl(3) | 2.2507 |
| 3 | Al(1)-Cl(4) | 2.251 |
| 4 | Al(1)-N(5) | 1.8087 |
| 5 | N(5)-N(6) | 1.2021 |
| 6 | N(6)-N(7) | 1.1709 |

Table 7-b: Bond angles [°] for composition $Na^+[AlCl_3(N_3)]^-$

| | Bond angles | [°] |
|---|---|---|
| 1 | Cl(2) Al(1)-Cl(3) | 109.4173 |
| 2 | Cl(2) Al(1)-Cl(4) | 109.4134 |
| 3 | Cl(2) Al(1)-N(5) | 109.5476 |
| 4 | Cl(3) Al(1)-Cl(4) | 109.4175 |
| 5 | Cl(3) Al(1)-N(5) | 109.4902 |
| 6 | Cl(4) Al(1)-N(5) | 109.5412 |
| 7 | Al(1)-N(5)-N(6) | 179.2262 |

$$NaN_3 + AlCl_3 \rightarrow Na\,[AlCl_3\,(N_3)]$$

In the vibrational spectrum of this compound, the known bands of cation and anion were seen such as $\nu_{Al\text{-}N}$ that was found at 529cm$^{-1}$ and confirmed with literature data. In the Mass spectra Na $[AlCl_3(N_3)]$ complex peak related to m/e=198 has been observed.

Figure 9. Optimized molecular structures of Na $[AlCl_3(N_3)]$ complex: From the optimized structure of the title compounds, molecular parameters can be extracted. Molecular parameters can depict a useful representation of molecular structure. Therefore, we extracted important bond lengths and bond angles of computed complex and listed them in (Table 7-a, 7-b).

## CONCLUSION

$Na[AlCl_3(NO_3)]$ was provided by the reaction of $NaNO_3$ and $AlCl_3$ in acetonitrile solvent and $Na[AlCl_3(CH_3COO)]$ was prepared by the reaction of $NaCH_3COO$ and $AlCl_3$ in acetonitrile solvent, $Na[AlCl_3(N_3)]$ was prepared by the reaction of $NaN_3$ and $AlCl_3$ in acetonitrile solvent. Electronic and vibrational and Mass spectra of these two Aluminate-complexes were studied. These compounds were characterized by IR and UV/Visible and Mass techniques. Ligands $NO_3^-$, $CH_3COO^-$, $N_3^-$ in the basis state to belong to point group $D_3h$, $D_3h$, $D_8h$ respectively. The electronic spectra indicate herami geometry for the complexes.

## ACKNOWLEDGEMENT

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