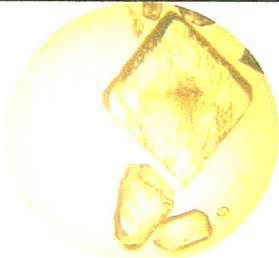
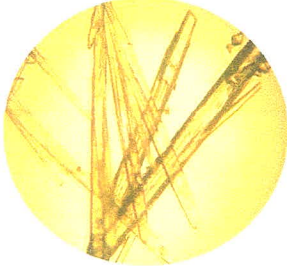

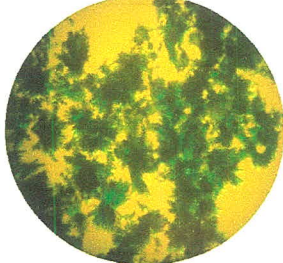
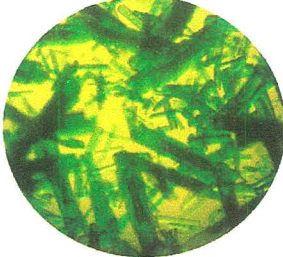
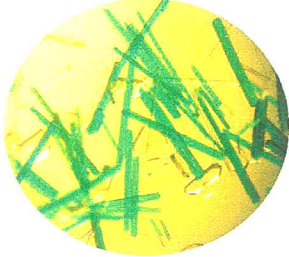
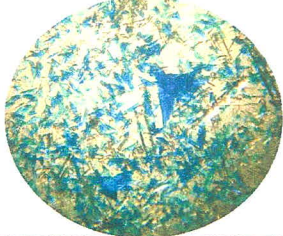


ภาคผนวก

ภาคผนวก 1 ข้อมูลกายภาพของสารประกอบเพิ่มเติม

| สารประกอบ | ภาพผลึกของงานวิจัยนี้ | ภาพผลึกของงานวิจัยอื่น ๆ |
|---|---|--|
| 1 |  | |
| 2 |  | |
| $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ |  | |
| 3 |  | |
| 4 |  |  |
| 5 |  | |

ภาคผนวก 2 ข้อมูลการเลี้ยวเบนของรังสีเอ็กซ์บนผลึกเดี่ยวของสารประกอบ

ภาคผนวก 2.1 สารประกอบ 1

Table 1.1 Crystal data and structure refinement for Compound 1.

| | |
|--|---|
| Identification code | compound 1 |
| Empirical formula | C7 H4 N2 O6 |
| Formula weight | 212.12 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | <i>C2/c</i> |
| Unit cell dimensions | $a = 21.059(3)$ Å $b = 8.7368(13)$ Å $c = 9.7553(14)$ Å $\alpha = \gamma = 90^\circ$ $\beta = 111.013(9)^\circ$ |
| Volume | $1675.5(4)$ Å ³ |
| Z | 8 |
| Density (calculated) | 1.682 Mg/m ³ |
| Absorption coefficient | 0.151 mm ⁻¹ |
| F(000) | 864 |
| Crystal size | $0.44 \times 0.32 \times 0.26$ mm ³ |
| θ range for data collection | 2.55 - 27.90° |
| Index ranges | $-27 \leq h \leq 27$, $-11 \leq k \leq 11$, $-12 \leq l \leq 12$ |
| Reflections collected | 6983 |
| Independent reflections | 1982 [R(int) = 0.0197] |
| Completeness to $\theta = 27.90^\circ$ | 99.2 % |
| Absorption correction | None |
| Max. and min. transmission | 0.9617 and 0.9364 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1982 / 0 / 153 |
| Goodness-of-fit on F^2 | 1.058 |
| Final R indices [$I > 2\sigma(I)$] | R1 = 0.0359, wR2 = 0.1005 |
| R indices (all data) | R1 = 0.0425, wR2 = 0.1060 |
| Extinction coefficient | 0.0088(10) |
| Largest diff. peak and hole | 0.234 and -0.184 e. Å ⁻³ |

Table 1.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| atom | x | y | z | $U(\text{eq})$ |
|-------|---------|---------|----------|----------------|
| O(26) | 354(1) | 3998(1) | 4218(1) | 59(1) |
| O(21) | 1953(1) | 6795(1) | 8264(1) | 53(1) |
| O(22) | 2309(1) | 5791(1) | 10521(1) | 53(1) |
| O(23) | 1716(1) | 468(1) | 11029(1) | 61(1) |
| O(24) | 1017(1) | -737(1) | 9181(2) | 78(1) |
| O(25) | -186(1) | 2095(2) | 4698(1) | 68(1) |
| N(21) | 1337(1) | 397(1) | 9750(1) | 47(1) |
| N(22) | 274(1) | 3032(1) | 5040(1) | 45(1) |
| C(21) | 1978(1) | 5729(1) | 9188(1) | 38(1) |
| C(22) | 1577(1) | 4328(1) | 8553(1) | 35(1) |
| C(23) | 1641(1) | 3047(2) | 9434(1) | 36(1) |
| C(24) | 1263(1) | 1763(1) | 8825(1) | 37(1) |
| C(25) | 814(1) | 1706(2) | 7391(2) | 38(1) |
| C(27) | 1137(1) | 4315(1) | 7100(1) | 36(1) |
| C(26) | 761(1) | 3011(2) | 6564(1) | 37(1) |

Table 1.3 Bond lengths [\AA] and angles [$^\circ$] for Compound 1.

| Bond length | [\AA] | Bond angles | [$^\circ$] |
|-------------------|------------------|-------------------|--------------|
| O(26)-N(22) | 1.2166(16) | C(21)-O(21)-H(21) | 114.4(14) |
| O(21)-C(21) | 1.2838(16) | O(24)-N(21)-O(23) | 124.20(12) |
| O(21)-H(21) | 1.02(3) | O(24)-N(21)-C(24) | 117.52(12) |
| O(22)-C(21) | 1.2372(16) | O(23)-N(21)-C(24) | 118.27(12) |
| O(23)-N(21) | 1.2178(17) | O(26)-N(22)-O(25) | 124.72(12) |
| O(24)-N(21) | 1.2143(17) | O(26)-N(22)-C(26) | 117.55(11) |
| O(25)-N(22) | 1.2196(16) | O(25)-N(22)-C(26) | 117.73(12) |
| N(21)-C(24) | 1.4704(17) | O(22)-C(21)-O(21) | 124.92(12) |
| N(22)-C(26) | 1.4736(16) | O(22)-C(21)-C(22) | 119.63(11) |
| C(21)-C(22) | 1.4897(17) | O(21)-C(21)-C(22) | 115.45(11) |
| C(22)-C(27) | 1.3876(17) | C(27)-C(22)-C(23) | 120.41(11) |
| C(22)-C(23) | 1.3881(18) | C(27)-C(22)-C(21) | 120.20(11) |
| C(23)-C(24) | 1.3799(18) | C(23)-C(22)-C(21) | 119.39(11) |
| C(23)-H(23) | 0.944(15) | C(24)-C(23)-C(22) | 118.47(12) |
| C(24)-C(25) | 1.3802(19) | C(24)-C(23)-H(23) | 120.5(9) |
| C(25)-C(26) | 1.3782(19) | C(22)-C(23)-H(23) | 121.1(9) |
| C(25)-H(25) | 0.937(17) | C(23)-C(24)-C(25) | 123.02(12) |
| C(27)-C(26) | 1.3787(18) | C(23)-C(24)-N(21) | 118.57(12) |
| C(27)-H(27) | 0.936(16) | C(25)-C(24)-N(21) | 118.40(11) |
| Bond angles | [$^\circ$] | C(26)-C(25)-C(24) | 116.46(11) |
| C(25)-C(26)-C(27) | 123.15(12) | C(26)-C(25)-H(25) | 121.7(10) |
| C(25)-C(26)-N(22) | 118.82(11) | C(24)-C(25)-H(25) | 121.9(10) |
| C(27)-C(26)-N(22) | 118.02(12) | C(26)-C(27)-C(22) | 118.47(12) |
| C(22)-C(27)-H(27) | 120.4(9) | C(26)-C(27)-H(27) | 121.1(9) |

Symmetry transformations used to generate equivalent atoms

Table 1.4 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2hk a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| O(26) | 68(1) | 64(1) | 37(1) | 4(1) | 11(1) | -3(1) |
| O(21) | 71(1) | 35(1) | 45(1) | 2(1) | 12(1) | -13(1) |
| O(22) | 67(1) | 47(1) | 38(1) | -5(1) | 11(1) | -18(1) |
| O(23) | 76(1) | 52(1) | 50(1) | 15(1) | 17(1) | 1(1) |
| O(24) | 113(1) | 43(1) | 72(1) | 4(1) | 26(1) | -27(1) |
| O(25) | 50(1) | 88(1) | 56(1) | -11(1) | 8(1) | -25(1) |
| N(21) | 59(1) | 36(1) | 52(1) | 4(1) | 26(1) | -3(1) |
| N(22) | 40(1) | 53(1) | 39(1) | -7(1) | 11(1) | -3(1) |
| C(21) | 44(1) | 33(1) | 36(1) | -2(1) | 14(1) | -3(1) |
| C(22) | 37(1) | 32(1) | 36(1) | -3(1) | 15(1) | -2(1) |
| C(23) | 38(1) | 36(1) | 34(1) | -1(1) | 14(1) | -1(1) |
| C(24) | 42(1) | 32(1) | 41(1) | 1(1) | 21(1) | -1(1) |
| C(25) | 40(1) | 35(1) | 43(1) | -8(1) | 19(1) | -7(1) |
| C(27) | 39(1) | 34(1) | 37(1) | 1(1) | 15(1) | 0(1) |
| C(26) | 35(1) | 41(1) | 35(1) | -5(1) | 13(1) | -2(1) |

Table 1.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 1.

| | x | y | z | U(eq) |
|-------|----------|----------|-----------|--------|
| H(23) | 1930(8) | 3053(17) | 10429(17) | 41(4) |
| H(25) | 567(8) | 818(19) | 6992(17) | 46(4) |
| H(27) | 1083(8) | 5191(18) | 6516(17) | 42(4) |
| H(21) | 2241(12) | 7730(30) | 8710(30) | 107(8) |

Table 1.6 Torsion angles [°] for Compound 1.

| Torsion angles | [°] | Torsion angles | [°] |
|-------------------------|-------------|-------------------------|-------------|
| O(22)-C(21)-C(22)-C(27) | 171.74(12) | C(23)-C(24)-C(25)-C(26) | 0.67(19) |
| O(21)-C(21)-C(22)-C(27) | -8.91(18) | N(21)-C(24)-C(25)-C(26) | 179.96(11) |
| O(22)-C(21)-C(22)-C(23) | -7.22(19) | C(23)-C(22)-C(27)-C(26) | 0.64(18) |
| O(21)-C(21)-C(22)-C(23) | 172.13(12) | C(21)-C(22)-C(27)-C(26) | -178.32(12) |
| C(27)-C(22)-C(23)-C(24) | 0.86(18) | C(24)-C(25)-C(26)-C(27) | 0.95(19) |
| C(21)-C(22)-C(23)-C(24) | 179.82(12) | C(24)-C(25)-C(26)-N(22) | -178.07(11) |
| C(22)-C(23)-C(24)-C(25) | -1.55(19) | C(22)-C(27)-C(26)-C(25) | -1.59(19) |
| C(22)-C(23)-C(24)-N(21) | 179.15(11) | C(22)-C(27)-C(26)-N(22) | 177.43(11) |
| O(24)-N(21)-C(24)-C(23) | -177.68(14) | O(26)-N(22)-C(26)-C(25) | -161.23(13) |
| O(23)-N(21)-C(24)-C(23) | 1.81(19) | O(25)-N(22)-C(26)-C(25) | 19.70(18) |
| O(24)-N(21)-C(24)-C(25) | 2.99(19) | O(26)-N(22)-C(26)-C(27) | 19.71(18) |
| O(23)-N(21)-C(24)-C(25) | -177.51(13) | O(25)-N(22)-C(26)-C(27) | -159.36(13) |

Symmetry transformations used to generate equivalent atoms

Table 1.7 Hydrogen bonds for Compound 1 [Å and °].

| D-H | d(D-H) | d(H..A) | <DHA | d(D..A) | A |
|---------|--------|---------|--------|---------|----------------------------|
| O21-H21 | 1.019 | 1.617 | 177.87 | 2.636 | O22 [-x+1/2, -y+3/2, -z+2] |

ภาคผนวก 2.2 ตารางประกอบ 1

Table 2.1 Crystal data and structure refinement for Compound 2

| | |
|--|--|
| Identification code | compound 2 |
| Empirical formula | C ₇ H ₆ O ₃ |
| Formula weight | 138.12 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | <i>P2(1)/c</i> |
| Unit cell dimensions | $a = 4.9067(8) \text{ \AA}$ $\alpha = 90^\circ$ $b = 11.218(2) \text{ \AA}$ $\beta = 90.806(10)^\circ$ $c = 11.537(2) \text{ \AA}$ $\gamma = 90^\circ$ |
| Volume | 635.0(2) Å ³ |
| Z | 4 |
| Density (calculated) | 1.445 Mg/m ³ |
| Absorption coefficient | 0.114 mm ⁻¹ |
| F(000) | 228 |
| Crystal size | 0.56 x 0.16 x 0.12 mm ³ |
| θ range for data collection | 3.53 - 26.09° |
| Index ranges | -6 ≤ h ≤ 5, -12 ≤ k ≤ 13, -14 ≤ l ≤ 13 |
| Reflections collected | 3145 |
| Independent reflections | 1246 [R(int) = 0.0176] |
| Completeness to $\theta = 27.90^\circ$ | 98.9 % |
| Absorption correction | None |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1246 / 0 / 116 |
| Goodness-of-fit on F^2 | 1.031 |
| Final R indices [$I > 2\sigma(I)$] | R1 = 0.0336, wR2 = 0.0866 |
| R indices (all data) | R1 = 0.0476, wR2 = 0.0955 |
| Extinction coefficient | 0.014(5) |
| Largest diff. peak and hole | 0.141-0.135 e. Å ⁻³ |

Table 2.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 2. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|---------|---------|---------|----------------|
| O(11) | 1627(2) | 3624(1) | 5504(1) | 49(1) |
| O(12) | 2300(2) | 4833(1) | 4010(1) | 45(1) |
| O(13) | 6019(2) | 4289(1) | 2495(1) | 59(1) |
| C(11) | 2861(3) | 3909(1) | 4547(1) | 36(1) |
| C(12) | 4944(3) | 3075(1) | 4163(1) | 36(1) |
| C(13) | 6397(3) | 3304(1) | 3154(1) | 41(1) |
| C(14) | 8369(3) | 2494(2) | 2796(2) | 52(1) |
| C(15) | 8856(3) | 1479(2) | 3426(2) | 56(1) |
| C(16) | 7423(3) | 1240(1) | 4419(2) | 56(1) |
| C(17) | 5487(3) | 2032(1) | 4785(1) | 47(1) |

Table 2.3 Bond lengths [\AA] and angles [$^\circ$] for Compound 2.

| Bond lengths [\AA] | [\AA] | Bond angles | [$^\circ$] |
|-------------------------------|------------------|-------------------|--------------|
| O(11)-C(11) | 1.3066(16) | O(12)-C(11)-C(12) | 122.53(12) |
| O(11)-H(11) | 0.96(2) | O(11)-C(11)-C(12) | 115.77(12) |
| O(12)-C(11) | 1.2365(15) | C(17)-C(12)-C(13) | 119.11(13) |
| O(13)-C(13) | 1.3533(18) | C(17)-C(12)-C(11) | 120.70(12) |
| O(13)-H(13) | 0.93(2) | C(13)-C(12)-C(11) | 120.18(12) |
| C(11)-C(12) | 1.4590(18) | O(13)-C(13)-C(14) | 117.11(14) |
| C(12)-C(17) | 1.3963(19) | O(13)-C(13)-C(12) | 123.43(12) |
| C(12)-C(13) | 1.397(2) | C(14)-C(13)-C(12) | 119.45(14) |
| C(13)-C(14) | 1.394(2) | C(15)-C(14)-C(13) | 120.05(15) |
| C(14)-C(15) | 1.370(2) | C(15)-C(14)-H(14) | 121.2(11) |
| C(14)-H(14) | 0.94(2) | C(13)-C(14)-H(14) | 118.7(11) |
| C(15)-C(16) | 1.379(3) | C(14)-C(15)-C(16) | 120.98(15) |
| C(15)-H(15) | 0.983(18) | C(14)-C(15)-H(15) | 118.2(11) |
| C(16)-C(17) | 1.371(2) | C(16)-C(15)-H(15) | 120.8(11) |
| C(16)-H(16) | 0.936(18) | C(17)-C(16)-C(15) | 119.60(16) |
| C(17)-H(17) | 0.968(17) | C(17)-C(16)-H(16) | 118.5(11) |
| | | C(15)-C(16)-H(16) | 121.9(11) |
| | | C(16)-C(17)-C(12) | 120.80(15) |
| | | C(16)-C(17)-H(17) | 120.1(10) |
| | | C(12)-C(17)-H(17) | 119.1(10) |
| | | C(11)-O(11)-H(11) | 109.7(11) |
| | | C(13)-O(13)-H(13) | 105.7(14) |
| | | O(12)-C(11)-O(11) | 121.70(12) |

Symmetry transformations used to generate equivalent atoms:

Table 2.4 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| O(11) | 51(1) | 48(1) | 50(1) | 9(1) | 20(1) | 11(1) |
| O(12) | 47(1) | 40(1) | 48(1) | 6(1) | 14(1) | 9(1) |
| O(13) | 68(1) | 60(1) | 51(1) | 8(1) | 23(1) | 15(1) |
| C(11) | 35(1) | 37(1) | 38(1) | -2(1) | 3(1) | -3(1) |
| C(12) | 33(1) | 35(1) | 41(1) | -5(1) | 0(1) | 1(1) |
| C(13) | 42(1) | 42(1) | 40(1) | -7(1) | 2(1) | 1(1) |
| C(14) | 47(1) | 61(1) | 48(1) | -16(1) | 9(1) | 8(1) |
| C(15) | 46(1) | 53(1) | 68(1) | -21(1) | -2(1) | 12(1) |
| C(16) | 52(1) | 43(1) | 73(1) | -1(1) | -4(1) | 11(1) |
| C(17) | 44(1) | 44(1) | 53(1) | 2(1) | 2(1) | 2(1) |

Table 2.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 2.

| | x | y | z | U(eq) |
|-------|-----------|----------|----------|--------|
| H(13) | 4650(40) | 4730(20) | 2857(19) | 103(8) |
| H(14) | 9340(40) | 2659(16) | 2114(17) | 70(5) |
| H(15) | 10290(40) | 936(15) | 3164(15) | 69(5) |
| H(16) | 7780(40) | 566(17) | 4874(15) | 72(6) |
| H(17) | 4440(30) | 1863(14) | 5472(15) | 56(5) |
| H(11) | 240(40) | 4201(17) | 5664(16) | 82(6) |

Table 2.6 Torsion angles [$^\circ$] for Compound 2.

| Torsion angles | [$^\circ$] | Torsion angles | [$^\circ$] |
|-------------------------|--------------|-------------------------|--------------|
| O(12)-C(11)-C(12)-C(17) | -179.05(13) | C(11)-C(12)-C(13)-C(14) | -179.60(13) |
| O(11)-C(11)-C(12)-C(17) | 1.47(19) | O(13)-C(13)-C(14)-C(15) | 179.87(14) |
| O(12)-C(11)-C(12)-C(13) | 0.0(2) | C(12)-C(13)-C(14)-C(15) | 0.5(2) |
| O(11)-C(11)-C(12)-C(13) | -179.48(12) | C(13)-C(14)-C(15)-C(16) | -0.1(3) |
| C(17)-C(12)-C(13)-O(13) | -179.88(13) | C(14)-C(15)-C(16)-C(17) | -0.2(3) |
| C(11)-C(12)-C(13)-O(13) | 1.1(2) | C(15)-C(16)-C(17)-C(12) | 0.1(2) |
| C(17)-C(12)-C(13)-C(14) | -0.5(2) | C(13)-C(12)-C(17)-C(16) | 0.2(2) |

Symmetry transformations used to generate equivalent atoms

Table 2.7 Hydrogen bonds for Compound 2 [\AA and $^\circ$].

| D-H | d(D-H) | d(H..A) | \angle DHA | d(D..A) | A |
|---------|--------|---------|--------------|---------|--------------------------|
| O13-H13 | 0.932 | 1.779 | 148.02 | 2.617 | O12 |
| O11-H11 | 0.959 | 1.698 | 177.02 | 2.656 | O12 [$-x, -y+1, -z+1$] |

ภาคผนวก 2.3 ตารางประกอบ 3

Table 3.1 Crystal data and structure refinement for Compound 3.

| | |
|---|--|
| Identification code | compound 3 |
| Empirical formula | C ₄₂ H ₃₂ Cu ₂ O ₁₂ |
| Formula weight | 855.76 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | <i>P2(1)/n</i> |
| Unit cell dimensions | <i>a</i> = 10.7755(3) Å <i>b</i> = 11.7248(4) Å <i>c</i> = 15.2284(5) Å $\alpha = \gamma = 90^\circ$ $\beta = 91.1950(10)^\circ$ |
| Volume | 1923.55(11) Å ³ |
| <i>Z</i> | 2 |
| Density (calculated) | 1.477 Mg/m ³ |
| Absorption coefficient | 1.170 mm ⁻¹ |
| F(000) | 876 |
| Crystal size | 0.40 x 0.34 x 0.30 mm ³ |
| θ range for data collection | 2.19 - 28.30° |
| Index ranges | -13 ≤ <i>h</i> ≤ 14, -15 ≤ <i>k</i> ≤ 15, -20 ≤ <i>l</i> ≤ 20 |
| Reflections collected | 16124 |
| Independent reflections | 4738 [R(int) = 0.0200] |
| Completeness to $\theta = 28.30^\circ$ | 98.7 % |
| Max. and min. transmission | 0.7204 and 0.6518 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4738 / 0 / 254 |
| Goodness-of-fit on F^2 | 1.019 |
| Final R indices [<i>I</i> > 2 σ (<i>I</i>)] | R1 = 0.0272, wR2 = 0.0721 |
| R indices (all data) | R1 = 0.0368, wR2 = 0.0783 |
| Largest diff. peak and hole | 0.317 and -0.183 e. Å ⁻³ |

Table 3.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 3. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | X | Y | Z | U(eq) |
|-------|---------|---------|----------|-------|
| Cu(1) | 5177(1) | 1065(1) | -209(1) | 32(1) |
| O(11) | 6854(1) | 501(1) | -547(1) | 43(1) |
| O(12) | 3471(1) | 1302(1) | 161(1) | 44(1) |
| O(21) | 5765(1) | 1199(1) | 1009(1) | 42(1) |
| O(22) | 5452(1) | -627(1) | 1367(1) | 45(1) |
| O(31) | 5683(1) | 2801(1) | -603(1) | 47(1) |
| O(32) | 7597(1) | 2515(1) | -1079(1) | 73(1) |
| C(11) | 2796(1) | 526(1) | 458(1) | 36(1) |
| C(12) | 1510(2) | 835(2) | 708(1) | 40(1) |
| C(13) | 1037(2) | 1881(2) | 448(2) | 59(1) |
| C(14) | -163(2) | 2181(2) | 637(2) | 74(1) |
| C(15) | -895(2) | 1461(2) | 1101(2) | 72(1) |
| C(16) | -429(2) | 433(3) | 1379(2) | 79(1) |
| C(17) | 774(2) | 107(2) | 1177(2) | 63(1) |
| C(21) | 5813(1) | 372(1) | 1535(1) | 36(1) |
| C(22) | 6369(2) | 588(2) | 2426(1) | 39(1) |
| C(23) | 6727(2) | 1674(2) | 2675(1) | 54(1) |
| C(24) | 7315(2) | 1857(2) | 3478(2) | 68(1) |
| C(25) | 7536(2) | 962(2) | 4039(2) | 67(1) |
| C(26) | 7170(2) | -118(2) | 3804(1) | 68(1) |
| C(27) | 6589(2) | -317(2) | 2996(1) | 54(1) |
| C(31) | 6609(2) | 3155(2) | -951(1) | 41(1) |
| C(32) | 6749(2) | 4343(2) | -1263(1) | 43(1) |
| C(33) | 7825(2) | 4719(2) | -1652(2) | 61(1) |
| C(34) | 7913(3) | 5836(2) | -1930(2) | 75(1) |
| C(35) | 6947(3) | 6575(2) | -1815(2) | 70(1) |
| C(36) | 5879(2) | 6210(2) | -1425(2) | 62(1) |
| C(37) | 5770(2) | 5092(2) | -1154(1) | 51(1) |

Table 3.3 Bond lengths [\AA] and angles [$^\circ$] for Compound 3.

| Bond lengths | [\AA] | Bond angles | [$^\circ$] |
|---------------|------------------|---------------------|--------------|
| Cu(1)-O(22)#1 | 1.9450(12) | C(11)-O(12)-Cu(1) | 123.82(11) |
| Cu(1)-O(21) | 1.9537(12) | C(21)-O(21)-Cu(1) | 123.39(11) |
| Cu(1)-O(12) | 1.9546(12) | C(21)-O(22)-Cu(1)#1 | 121.98(11) |
| Cu(1)-O(11) | 2.0009(11) | C(31)-O(31)-Cu(1) | 130.38(12) |
| Cu(1)-O(31) | 2.1944(12) | C(31)-O(32)-H(32) | 109.5 |
| Cu(1)-Cu(1)#1 | 2.6073(4) | O(12)-C(11)-O(11)#1 | 123.59(15) |
| O(11)-C(11)#1 | 1.268(2) | O(12)-C(11)-C(12) | 117.70(15) |
| O(12)-C(11) | 1.255(2) | O(11)#1-C(11)-C(12) | 118.71(15) |
| O(21)-C(21) | 1.258(2) | C(17)-C(12)-C(13) | 119.07(17) |
| O(22)-C(21) | 1.259(2) | C(17)-C(12)-C(11) | 122.10(16) |
| O(22)-Cu(1)#1 | 1.9451(12) | C(13)-C(12)-C(11) | 118.82(17) |

Table 3.3 Bond lengths [\AA] and angles [$^{\circ}$] for Compound 3. (ต่อ)

| Bond lengths | [\AA] | Bond angles | [$^{\circ}$] |
|---------------------|------------------|--------------------|----------------|
| O(31)-C(31) | 1.212(2) | C(14)-C(13)-C(12) | 120.6(2) |
| O(32)-C(31) | 1.320(2) | C(14)-C(13)-H(13A) | 119.7 |
| O(32)-H(32) | 0.8200 | C(12)-C(13)-H(13A) | 119.7 |
| C(11)-O(11)#1 | 1.268(2) | C(15)-C(14)-C(13) | 120.4(2) |
| C(11)-C(12) | 1.489(2) | C(15)-C(14)-H(14A) | 119.8 |
| C(12)-C(17) | 1.376(3) | C(13)-C(14)-H(14A) | 119.8 |
| C(12)-C(13) | 1.383(3) | C(14)-C(15)-C(16) | 119.6(2) |
| C(13)-C(14) | 1.376(3) | C(14)-C(15)-H(15A) | 120.2 |
| C(13)-H(13A) | 0.9300 | C(16)-C(15)-H(15A) | 120.2 |
| C(14)-C(15) | 1.362(4) | C(15)-C(16)-C(17) | 120.7(2) |
| C(14)-H(14A) | 0.9300 | C(15)-C(16)-H(16A) | 119.7 |
| C(15)-C(16) | 1.369(4) | C(17)-C(16)-H(16A) | 119.7 |
| C(15)-H(15A) | 0.9300 | C(12)-C(17)-C(16) | 119.6(2) |
| C(16)-C(17) | 1.392(3) | C(12)-C(17)-H(17A) | 120.2 |
| C(16)-H(16A) | 0.9300 | C(16)-C(17)-H(17A) | 120.2 |
| C(17)-H(17A) | 0.9300 | O(21)-C(21)-O(22) | 125.45(15) |
| C(21)-C(22) | 1.494(2) | O(21)-C(21)-C(22) | 117.29(15) |
| C(22)-C(23) | 1.381(3) | O(22)-C(21)-C(22) | 117.25(15) |
| C(22)-C(27) | 1.388(3) | C(23)-C(22)-C(27) | 119.36(17) |
| C(23)-C(24) | 1.383(3) | C(23)-C(22)-C(21) | 120.63(16) |
| C(23)-H(23A) | 0.9300 | C(27)-C(22)-C(21) | 119.92(17) |
| C(24)-C(25) | 1.370(3) | C(22)-C(23)-C(24) | 120.4(2) |
| C(24)-H(24A) | 0.9300 | C(22)-C(23)-H(23A) | 119.8 |
| C(25)-C(26) | 1.371(3) | C(24)-C(23)-H(23A) | 119.8 |
| C(25)-H(25A) | 0.9300 | C(25)-C(24)-C(23) | 120.2(2) |
| C(26)-C(27) | 1.389(3) | C(25)-C(24)-H(24A) | 119.9 |
| C(26)-H(26A) | 0.9300 | C(23)-C(24)-H(24A) | 119.9 |
| C(27)-H(27A) | 0.9300 | C(24)-C(25)-C(26) | 120.0(2) |
| C(31)-C(32) | 1.481(2) | C(24)-C(25)-H(25A) | 120.0 |
| C(32)-C(37) | 1.384(3) | C(26)-C(25)-H(25A) | 120.0 |
| C(32)-C(33) | 1.385(3) | C(25)-C(26)-C(27) | 120.5(2) |
| C(33)-C(34) | 1.380(3) | C(25)-C(26)-H(26A) | 119.8 |
| C(33)-H(33A) | 0.9300 | C(27)-C(26)-H(26A) | 119.8 |
| C(34)-C(35) | 1.369(4) | C(22)-C(27)-C(26) | 119.6(2) |
| C(34)-H(34A) | 0.9300 | C(22)-C(27)-H(27A) | 120.2 |
| C(35)-C(36) | 1.374(4) | C(26)-C(27)-H(27A) | 120.2 |
| C(35)-H(35A) | 0.9300 | O(31)-C(31)-O(32) | 122.96(16) |
| C(36)-C(37) | 1.380(3) | O(31)-C(31)-C(32) | 123.50(16) |
| C(36)-H(36A) | 0.9300 | O(32)-C(31)-C(32) | 113.54(16) |
| C(37)-H(37A) | 0.9300 | C(37)-C(32)-C(33) | 119.79(18) |
| Bond angles | [$^{\circ}$] | C(37)-C(32)-C(31) | 118.35(17) |
| O(22)#1-Cu(1)-O(21) | 169.11(5) | C(33)-C(32)-C(31) | 121.86(18) |
| O(22)#1-Cu(1)-O(12) | 89.25(6) | C(34)-C(33)-C(32) | 119.7(2) |
| O(21)-Cu(1)-O(12) | 90.18(6) | C(34)-C(33)-H(33A) | 120.1 |
| O(22)#1-Cu(1)-O(11) | 88.82(5) | C(32)-C(33)-H(33A) | 120.1 |
| O(21)-Cu(1)-O(11) | 89.64(5) | C(35)-C(34)-C(33) | 120.3(2) |
| O(12)-Cu(1)-O(11) | 168.82(5) | C(35)-C(34)-H(34A) | 119.9 |

Table 3.3 Bond lengths [Å] and angles [°] for Compound 3. (ต่อ)

| Bond angles | [°] | Bond angles | [°] |
|---------------------|------------|--------------------|-------|
| O(12)-Cu(1)-O(31) | 100.80(5) | C(34)-C(35)-H(35A) | 119.9 |
| O(11)-Cu(1)-O(31) | 90.33(5) | C(36)-C(35)-H(35A) | 119.9 |
| O(12)-Cu(1)-Cu(1)#1 | 85.54(4) | C(37)-C(36)-H(36A) | 119.9 |
| O(31)-Cu(1)-Cu(1)#1 | 173.66(3) | C(36)-C(37)-H(37A) | 120.1 |
| C(11)#1-O(11)-Cu(1) | 123.70(11) | C(32)-C(37)-H(37A) | 120.1 |

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table 3.4 Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for Compound 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}] U^{11}$

| | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} | U^{22} |
|-------|----------|----------|----------|----------|----------|----------|
| Cu(1) | 32(1) | 29(1) | 34(1) | 1(1) | -1(1) | 1(1) |
| O(11) | 37(1) | 37(1) | 55(1) | 4(1) | 8(1) | 6(1) |
| O(12) | 35(1) | 38(1) | 59(1) | 4(1) | 6(1) | 6(1) |
| O(21) | 50(1) | 41(1) | 36(1) | 0(1) | -6(1) | 0(1) |
| O(22) | 55(1) | 42(1) | 39(1) | 0(1) | -9(1) | -6(1) |
| O(31) | 49(1) | 36(1) | 57(1) | 5(1) | 9(1) | 2(1) |
| O(32) | 58(1) | 43(1) | 118(1) | 17(1) | 31(1) | 7(1) |
| C(11) | 32(1) | 40(1) | 35(1) | -2(1) | -2(1) | 4(1) |
| C(12) | 33(1) | 45(1) | 41(1) | -6(1) | 1(1) | 5(1) |
| C(13) | 46(1) | 51(1) | 81(2) | 5(1) | 12(1) | 11(1) |
| C(14) | 51(1) | 66(1) | 106(2) | 0(1) | 10(1) | 23(1) |
| C(15) | 41(1) | 85(2) | 91(2) | -14(1) | 14(1) | 13(1) |
| C(16) | 53(1) | 90(2) | 95(2) | 10(2) | 28(1) | 1(1) |
| C(17) | 49(1) | 65(1) | 74(1) | 13(1) | 16(1) | 10(1) |
| C(21) | 30(1) | 42(1) | 36(1) | -3(1) | 0(1) | 2(1) |
| C(22) | 34(1) | 49(1) | 35(1) | -3(1) | -2(1) | 0(1) |
| C(23) | 66(1) | 50(1) | 45(1) | -3(1) | -9(1) | -1(1) |
| C(24) | 85(2) | 63(1) | 54(1) | -16(1) | -16(1) | -9(1) |
| C(25) | 71(2) | 83(2) | 46(1) | -10(1) | -21(1) | 2(1) |
| C(26) | 81(2) | 72(2) | 49(1) | 8(1) | -22(1) | 2(1) |
| C(27) | 59(1) | 54(1) | 47(1) | 3(1) | -12(1) | -5(1) |
| C(31) | 45(1) | 36(1) | 42(1) | -2(1) | 1(1) | -1(1) |
| C(32) | 55(1) | 36(1) | 39(1) | -1(1) | 0(1) | -3(1) |
| C(33) | 63(1) | 45(1) | 74(1) | 4(1) | 12(1) | -6(1) |
| C(34) | 87(2) | 53(1) | 85(2) | 11(1) | 16(1) | -20(1) |
| C(35) | 106(2) | 38(1) | 64(1) | 9(1) | -2(1) | -10(1) |
| C(36) | 86(2) | 42(1) | 58(1) | 1(1) | -7(1) | 13(1) |

Table 3.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 3.

| | X | Y | Z | U(eq) |
|--------|-------|-------|-------|-------|
| H(32) | 7454 | 1860 | -923 | 109 |
| H(13A) | 1534 | 2387 | 144 | 71 |
| H(14A) | -477 | 2879 | 446 | 89 |
| H(15A) | -1705 | 1667 | 1228 | 87 |
| H(16A) | -922 | -52 | 1707 | 95 |
| H(17A) | 1078 | -599 | 1358 | 75 |
| H(23A) | 6572 | 2286 | 2300 | 64 |
| H(24A) | 7562 | 2590 | 3638 | 81 |
| H(25A) | 7934 | 1088 | 4578 | 81 |
| H(26A) | 7313 | -722 | 4190 | 81 |
| H(27A) | 6350 | -1052 | 2837 | 64 |
| H(33A) | 8487 | 4220 | -1725 | 73 |
| H(34A) | 8633 | 6088 | -2196 | 90 |
| H(35A) | 7013 | 7327 | -2003 | 84 |
| H(36A) | 5229 | 6717 | -1344 | 75 |
| H(37A) | 5042 | 4842 | -899 | 61 |

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Compound 3 [\AA and $^\circ$].

| D-H | d(D-H) | d(H..A) | \angle DHA | d(D..A) | A |
|---------|--------|---------|--------------|---------|-----|
| O32-H32 | 0.820 | 1.817 | 169.57 | 2.627 | O11 |

ภาคผนวก 2.4 ตารางประกอบ 4

Table 4.1 Crystal data and structure refinement for Compound 4

| | |
|--|--|
| Identification code | compound 4 |
| Empirical formula | C ₁₄ H ₁₆ Cu N ₂ O ₁₃ |
| Formula weight | 483.84 |
| Temperature | 298 K |
| Wavelength | 0.71073 Å |
| Crystal system | Orthorhombic |
| Space group | <i>Pna2(1)</i> |
| Unit cell dimensions | $a = 7.2952(6)$ Å $\alpha = 90^\circ$ $b = 34.943(3)$ Å $\beta = 90^\circ$ $c = 7.3779(6)$ Å $\gamma = 90^\circ$ |
| Volume | 1880.8(3) Å ³ |
| Z | 4 |
| Density (calculated) | 1.709 Mg/m ³ |
| Absorption coefficient | 1.236 mm ⁻¹ |
| F(000) | 988 |
| Crystal size | 0.328 x 0.13 x 0.097 mm ³ |
| θ range for data collection | 1.17 - 28.34 ° |
| Index ranges | -9 ≤ h ≤ 9, -46 ≤ k ≤ 46, -9 ≤ l ≤ 9 |
| Reflections collected | 21887 |
| Independent reflections | 4681 [R(int) = 0.0275] |
| Completeness to $\theta = 27.90^\circ$ | 100.0 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.887 and 0.825 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4681 / 1 / 303 |
| Goodness-of-fit on F^2 | 1.043 |
| Final R indices [$I > 2\sigma(I)$] | R1 = 0.0289, wR2 = 0.0685 |
| R indices (all data) | R1 = 0.0376, wR2 = 0.0723 |
| Largest diff. peak and hole | 0.339 and -0.272 e. Å ⁻³ |

Table 4.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | X | Y | Z | U(eq) |
|-------|---------|---------|----------|-------|
| Cu(1) | 3952(1) | 7488(1) | -585(1) | 30(1) |
| O(1) | 2292(3) | 7498(1) | 1478(3) | 41(1) |
| O(2) | 5785(3) | 7471(1) | -2531(3) | 40(1) |
| O(3) | 5322(3) | 6813(1) | 5516(3) | 55(1) |
| O(4) | 6386(4) | 8092(1) | 5624(3) | 56(1) |
| O(11) | 4001(2) | 8037(1) | -680(3) | 34(1) |
| O(12) | 5310(2) | 8131(1) | 1996(2) | 40(1) |
| O(13) | 3057(2) | 8606(1) | -2661(3) | 51(1) |
| O(21) | 3828(2) | 6940(1) | -675(3) | 37(1) |
| O(22) | 5402(2) | 6852(1) | 1872(2) | 38(1) |
| O(26) | 1906(3) | 5850(1) | -4189(3) | 69(1) |
| O(25) | 1782(3) | 5290(1) | -2996(3) | 73(1) |
| O(23) | 5543(3) | 5545(1) | 4380(3) | 66(1) |
| O(24) | 4125(3) | 5091(1) | 3016(3) | 74(1) |
| N(22) | 2159(3) | 5628(1) | -2950(3) | 47(1) |
| N(21) | 4656(3) | 5421(1) | 3132(3) | 45(1) |
| C(11) | 4520(3) | 8255(1) | 634(3) | 29(1) |
| C(12) | 4128(3) | 8670(1) | 426(3) | 29(1) |
| C(13) | 4478(3) | 8915(1) | 1876(3) | 35(1) |
| C(14) | 4152(3) | 9304(1) | 1733(4) | 42(1) |
| C(15) | 3464(3) | 9451(1) | 126(4) | 45(1) |
| C(16) | 3087(3) | 9215(1) | -1321(3) | 40(1) |
| C(17) | 3423(3) | 8823(1) | -1178(3) | 34(1) |
| C(21) | 4477(3) | 6732(1) | 576(3) | 28(1) |
| C(22) | 4108(3) | 6312(1) | 415(3) | 28(1) |
| C(23) | 4563(3) | 6064(1) | 1819(3) | 30(1) |
| C(24) | 4185(3) | 5681(1) | 1631(3) | 33(1) |
| C(25) | 3386(3) | 5527(1) | 99(3) | 36(1) |
| C(26) | 2987(3) | 5778(1) | -1289(3) | 33(1) |
| C(27) | 3304(3) | 6168(1) | -1154(3) | 31(1) |

Table 4.3 Bond lengths [\AA] and angles [$^\circ$] for compound 4

| Bond lengths | [\AA] | Bond angles | [$^\circ$] |
|--------------|------------------|--------------------|--------------|
| Cu(1)-O(11) | 1.9174(12) | Cu(1)-O(2)-H(2B) | 106(2) |
| Cu(1)-O(11) | 1.9174(12) | Cu(1)-O(2)-H(2A) | 118(2) |
| Cu(1)-O(21) | 1.9189(12) | H(2B)-O(2)-H(2A) | 111(3) |
| Cu(1)-O(1) | 1.9453(19) | H(3B)-O(3)-H(3A) | 114(4) |
| Cu(1)-O(2) | 1.9629(19) | H(4B)-O(4)-H(4A) | 118(4) |
| O(1)-H(1A) | 0.74(3) | C(11)-O(11)-Cu(1) | 124.65(17) |
| O(1)-H(1B) | 0.70(3) | C(17)-O(13)-H(13A) | 109.5 |
| O(2)-H(2B) | 0.84(3) | C(21)-O(21)-Cu(1) | 122.03(17) |
| O(2)-H(2A) | 0.85(4) | O(26)-N(22)-O(25) | 124.4(2) |
| O(3)-H(3B) | 0.77(3) | O(26)-N(22)-C(26) | 117.80(18) |

Table 4.3 Bond lengths [Å] and angles [°] for compound 4 (ต่อ)

| Bond lengths | [Å] | Bond angles | [°] |
|-------------------|------------|-------------------|------------|
| O(3)-H(3A) | 0.87(5) | O(25)-N(22)-C(26) | 117.8(2) |
| O(4)-H(4B) | 0.75(4) | O(23)-N(21)-O(24) | 124.41(19) |
| O(4)-H(4A) | 0.88(4) | O(23)-N(21)-C(24) | 118.43(17) |
| O(11)-C(11) | 1.290(3) | O(24)-N(21)-C(24) | 117.2(2) |
| O(12)-C(11) | 1.237(2) | O(12)-C(11)-O(11) | 122.63(17) |
| O(13)-C(17) | 1.357(3) | O(12)-C(11)-C(12) | 121.06(17) |
| O(13)-H(13A) | 0.8200 | O(11)-C(11)-C(12) | 116.31(18) |
| O(21)-C(21) | 1.267(3) | C(13)-C(12)-C(17) | 118.78(17) |
| O(22)-C(21) | 1.244(2) | C(13)-C(12)-C(11) | 119.10(19) |
| O(26)-N(22) | 1.212(3) | C(17)-C(12)-C(11) | 122.12(19) |
| O(25)-N(22) | 1.214(2) | C(14)-C(13)-C(12) | 120.9(2) |
| O(23)-N(21) | 1.207(3) | C(14)-C(13)-H(13) | 119.5 |
| O(24)-N(21) | 1.218(2) | C(12)-C(13)-H(13) | 119.5 |
| N(22)-C(26) | 1.463(3) | C(13)-C(14)-C(15) | 119.4(2) |
| N(21)-C(24) | 1.473(3) | C(13)-C(14)-H(14) | 120.3 |
| C(11)-C(12) | 1.485(2) | C(15)-C(14)-H(14) | 120.3 |
| C(12)-C(13) | 1.395(3) | C(16)-C(15)-C(14) | 121.0(2) |
| C(12)-C(17) | 1.396(3) | C(16)-C(15)-H(15) | 119.5 |
| C(13)-C(14) | 1.383(3) | C(14)-C(15)-H(15) | 119.5 |
| C(13)-H(13) | 0.9300 | C(15)-C(16)-C(17) | 119.6(2) |
| C(14)-C(15) | 1.386(4) | C(15)-C(16)-H(16) | 120.2 |
| C(14)-H(14) | 0.9300 | C(17)-C(16)-H(16) | 120.2 |
| C(15)-C(16) | 1.375(4) | O(13)-C(17)-C(16) | 116.8(2) |
| C(15)-H(15) | 0.9300 | O(13)-C(17)-C(12) | 122.86(18) |
| C(16)-C(17) | 1.396(3) | C(16)-C(17)-C(12) | 120.3(2) |
| C(16)-H(16) | 0.9300 | O(22)-C(21)-O(21) | 124.65(17) |
| C(21)-C(22) | 1.498(2) | O(22)-C(21)-C(22) | 119.35(17) |
| C(22)-C(23) | 1.390(3) | O(21)-C(21)-C(22) | 115.98(18) |
| C(22)-C(27) | 1.391(3) | C(23)-C(22)-C(27) | 119.81(17) |
| C(23)-C(24) | 1.376(3) | C(23)-C(22)-C(21) | 120.52(19) |
| C(23)-H(23) | 0.9300 | C(27)-C(22)-C(21) | 119.66(18) |
| C(24)-C(25) | 1.380(3) | C(24)-C(23)-C(22) | 118.89(19) |
| C(25)-C(26) | 1.379(3) | C(24)-C(23)-H(23) | 120.6 |
| C(25)-H(25) | 0.9300 | C(22)-C(23)-H(23) | 120.6 |
| C(27)-H(27) | 0.9300 | C(23)-C(24)-N(21) | 118.6(2) |
| Bond angles | [°] | C(25)-C(24)-N(21) | 118.35(18) |
| O(11)-Cu(1)-O(21) | 175.58(14) | C(26)-C(25)-C(24) | 116.79(18) |
| O(11)-Cu(1)-O(21) | 175.58(14) | C(26)-C(25)-H(25) | 121.6 |
| O(11)-Cu(1)-O(1) | 91.32(8) | C(24)-C(25)-H(25) | 121.6 |
| O(21)-Cu(1)-O(1) | 90.87(8) | C(25)-C(26)-C(27) | 122.5(2) |
| O(11)-Cu(1)-O(2) | 89.54(8) | C(25)-C(26)-N(22) | 118.79(18) |
| O(1)-Cu(1)-O(2) | 175.47(9) | C(26)-C(27)-C(22) | 118.95(19) |
| Cu(1)-O(1)-H(1A) | 119(2) | C(26)-C(27)-H(27) | 120.5 |
| Cu(1)-O(1)-H(1B) | 113(3) | C(22)-C(27)-H(27) | 120.5 |
| H(1A)-O(1)-H(1B) | 116(4) | | |

Symmetry transformations used to generate equivalent atoms:

Table 4.4 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| Cu(1) | 47(1) | 17(1) | 26(1) | 0(1) | -1(1) | 1(1) |
| O(1) | 62(1) | 18(1) | 44(1) | 0(1) | 15(1) | 1(1) |
| O(2) | 60(1) | 27(1) | 34(1) | -1(1) | 7(1) | 1(1) |
| O(3) | 86(2) | 51(1) | 29(1) | -7(1) | -4(1) | 14(1) |
| O(4) | 77(2) | 49(1) | 41(1) | 9(1) | -7(1) | -5(1) |
| O(11) | 52(1) | 19(1) | 33(1) | -3(1) | -2(1) | -1(1) |
| O(12) | 57(1) | 30(1) | 34(1) | -2(1) | -8(1) | 8(1) |
| O(13) | 77(1) | 31(1) | 44(1) | -4(1) | -22(1) | 8(1) |
| O(21) | 60(1) | 19(1) | 31(1) | 4(1) | -2(1) | 3(1) |
| O(22) | 54(1) | 26(1) | 33(1) | -1(1) | -4(1) | -7(1) |
| O(26) | 97(2) | 68(1) | 43(1) | -13(1) | -21(1) | 5(1) |
| O(25) | 94(2) | 45(1) | 79(1) | -30(1) | -10(1) | -14(1) |
| O(23) | 83(1) | 66(1) | 55(1) | 27(1) | -20(1) | -5(1) |
| O(24) | 109(2) | 29(1) | 84(1) | 22(1) | 0(1) | -1(1) |
| N(22) | 50(1) | 44(1) | 47(1) | -19(1) | -1(1) | 3(1) |
| N(21) | 45(1) | 31(1) | 54(1) | 18(1) | 8(1) | 7(1) |
| C(11) | 36(1) | 21(1) | 32(1) | -2(1) | 2(1) | -1(1) |
| C(12) | 30(1) | 21(1) | 37(1) | -1(1) | -2(1) | 0(1) |
| C(13) | 37(1) | 29(1) | 41(1) | -5(1) | -1(1) | 2(1) |
| C(14) | 45(1) | 27(1) | 54(2) | -13(1) | 0(1) | 0(1) |
| C(15) | 44(1) | 24(1) | 68(2) | -2(1) | 4(1) | 2(1) |
| C(16) | 41(1) | 26(1) | 53(1) | 7(1) | -2(1) | 2(1) |
| C(17) | 37(1) | 26(1) | 37(1) | 0(1) | -2(1) | -2(1) |
| C(21) | 37(1) | 21(1) | 27(1) | 0(1) | 5(1) | 1(1) |
| C(22) | 33(1) | 22(1) | 31(1) | -1(1) | 2(1) | 1(1) |
| C(23) | 33(1) | 26(1) | 32(1) | 3(1) | 2(1) | 1(1) |
| C(24) | 33(1) | 26(1) | 39(1) | 7(1) | 5(1) | 4(1) |
| C(25) | 38(1) | 21(1) | 49(1) | -4(1) | 7(1) | 1(1) |
| C(26) | 33(1) | 27(1) | 39(1) | -10(1) | 2(1) | 1(1) |
| C(27) | 36(1) | 26(1) | 31(1) | 0(1) | 3(1) | 5(1) |

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 4

| | X | Y | Z | U(eq) |
|--------|----------|----------|-----------|---------|
| H(1A) | 1770(40) | 7675(8) | 1670(40) | 43(8) |
| H(1B) | 1820(40) | 7327(9) | 1600(40) | 46(9) |
| H(2B) | 5560(40) | 7271(8) | -3120(40) | 51(8) |
| H(2A) | 5870(40) | 7662(10) | -3230(50) | 62(10) |
| H(3B) | 5420(40) | 6803(6) | 4480(50) | 42(7) |
| H(4B) | 5860(50) | 8101(9) | 4750(60) | 76(12) |
| H(4A) | 7580(60) | 8125(9) | 5580(60) | 104(14) |
| H(13A) | 3297 | 8382 | -2443 | 76 |
| H(13) | 4937 | 8816 | 2954 | 42 |
| H(14) | 4392 | 9466 | 2706 | 51 |
| H(15) | 3253 | 9712 | 24 | 54 |
| H(16) | 2612 | 9316 | -2387 | 48 |
| H(23) | 5115 | 6157 | 2868 | 36 |
| H(25) | 3129 | 5267 | 7 | 43 |
| H(27) | 2983 | 6332 | -2098 | 37 |
| H(3A) | 5950(60) | 6642(12) | 6100(70) | 127(17) |

Table 6. Torsion angles [$^\circ$] for compound 4

| Torsion angles | [$^\circ$] | Torsion angles | [$^\circ$] |
|-------------------------|--------------|-------------------------|--------------|
| O(21)-Cu(1)-O(11)-C(11) | 178.2(9) | O(22)-C(21)-C(22)-C(23) | 9.1(3) |
| O(1)-Cu(1)-O(11)-C(11) | 58.57(17) | O(21)-C(21)-C(22)-C(23) | -172.20(19) |
| O(2)-Cu(1)-O(11)-C(11) | -116.98(17) | O(22)-C(21)-C(22)-C(27) | -170.89(19) |
| O(11)-Cu(1)-O(21)-C(21) | 173.7(9) | O(21)-C(21)-C(22)-C(27) | 7.8(3) |
| O(1)-Cu(1)-O(21)-C(21) | -66.68(18) | C(27)-C(22)-C(23)-C(24) | -0.8(3) |
| O(2)-Cu(1)-O(21)-C(21) | 108.82(18) | C(21)-C(22)-C(23)-C(24) | 179.25(18) |
| Cu(1)-O(11)-C(11)-O(12) | 11.6(3) | C(22)-C(23)-C(24)-C(25) | 0.7(3) |
| Cu(1)-O(11)-C(11)-C(12) | -168.74(13) | C(22)-C(23)-C(24)-N(21) | -179.47(18) |
| O(12)-C(11)-C(12)-C(13) | -7.0(3) | O(23)-N(21)-C(24)-C(23) | -8.3(3) |
| O(11)-C(11)-C(12)-C(13) | 173.36(19) | O(24)-N(21)-C(24)-C(23) | 172.1(2) |
| O(12)-C(11)-C(12)-C(17) | 172.8(2) | O(23)-N(21)-C(24)-C(25) | 171.6(2) |
| O(11)-C(11)-C(12)-C(17) | -6.8(3) | O(24)-N(21)-C(24)-C(25) | -8.1(3) |
| C(17)-C(12)-C(13)-C(14) | -0.5(3) | C(23)-C(24)-C(25)-C(26) | 0.8(3) |
| C(11)-C(12)-C(13)-C(14) | 179.3(2) | N(21)-C(24)-C(25)-C(26) | -179.07(18) |
| C(12)-C(13)-C(14)-C(15) | 0.1(3) | C(24)-C(25)-C(26)-C(27) | -2.2(3) |
| C(13)-C(14)-C(15)-C(16) | 0.5(4) | C(24)-C(25)-C(26)-N(22) | 179.30(19) |
| C(14)-C(15)-C(16)-C(17) | -0.8(4) | O(26)-N(22)-C(26)-C(25) | -176.3(2) |
| C(15)-C(16)-C(17)-O(13) | -178.8(2) | O(25)-N(22)-C(26)-C(25) | 3.3(3) |
| C(15)-C(16)-C(17)-C(12) | 0.3(3) | O(26)-N(22)-C(26)-C(27) | 5.2(3) |
| C(13)-C(12)-C(17)-O(13) | 179.4(2) | O(25)-N(22)-C(26)-C(27) | -175.3(2) |
| C(11)-C(12)-C(17)-O(13) | -0.4(3) | C(25)-C(26)-C(27)-C(22) | 2.1(3) |
| C(13)-C(12)-C(17)-C(16) | 0.3(3) | N(22)-C(26)-C(27)-C(22) | -179.37(19) |
| C(11)-C(12)-C(17)-C(16) | -179.5(2) | C(23)-C(22)-C(27)-C(26) | -0.6(3) |
| Cu(1)-O(21)-C(21)-O(22) | -7.5(3) | C(21)-C(22)-C(27)-C(26) | 179.39(19) |
| Cu(1)-O(21)-C(21)-C(22) | 173.87(13) | | |

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for ortho [\AA and $^\circ$].

| D-H | d(D-H) | d(H..A) | \angle DHA | d(D..A) | A |
|----------|--------|---------|--------------|---------|----------------------------|
| O1-H1A | 0.739 | 1.936 | 173.68 | 2.672 | O22 [x-1/2, -y+3/2, z] |
| O1-H1B | 0.698 | 1.961 | 175.58 | 2.658 | O12 [x-1/2, -y+3/2, z] |
| O2-H2B | 0.837 | 1.901 | 174.02 | 2.734 | O3 [x, y, z-1] |
| O2-H2A | 0.847 | 1.764 | 168.51 | 2.600 | O4 [x, y, z-1] |
| O3-H3B | 0.766 | 1.934 | 170.41 | 2.693 | O22 |
| O4-H4B | 0.754 | 2.071 | 160.44 | 2.793 | O12 |
| O4-H4A | 0.880 | 2.011 | 178.65 | 2.891 | O3 [x+1/2, -y+3/2, z] |
| O13-H13A | 0.820 | 1.846 | 145.33 | 2.564 | O11 |
| O3-H3A | 0.867 | 1.988 | 159.75 | 2.817 | O13 [x+1/2, -y+3/2, z+1] |

ภาคผนวก 2.5 สารประกอบ 4

Table 5.1 Crystal data and structure refinement for Compound 5

| | |
|--|--|
| Identification code | compound 5 |
| Empirical formula | C ₂₈ H ₃₂ Cu ₂ N ₄ O ₂₆ |
| Formula weight | 967.68 |
| Temperature | 298 K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | <i>P2(1)/c</i> |
| Unit cell dimensions | $a = 15.2492(9) \text{ \AA}$ $\alpha = 90^\circ$ $b = 6.9556(4) \text{ \AA}$ $\beta = 91.5920(10)^\circ$ $c = 17.3171(10) \text{ \AA}$ $\gamma = 90^\circ$ |
| Volume | 1836.07(18) ³ |
| Z | 2 |
| Density (calculated) | 1.750 Mg/m ³ |
| Absorption coefficient | 1.266 mm ⁻¹ |
| F(000) | 988 |
| Crystal size | 0.279 x 0.257 x 0.131 mm ³ |
| θ range for data collection | 1.34 - 28.32° |
| Index ranges | -20 ≤ h ≤ 20, -9 ≤ k ≤ 9, -23 ≤ l ≤ 23 |
| Reflections collected | 12882 |
| Independent reflections | 4582 [R(int) = 0.0233] |
| Completeness to $\theta = 28.32^\circ$ | 99.7 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.847 and 0.709 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4582 / 0 / 296 |
| Goodness-of-fit on F^2 | 0.928 |
| Final R indices [$I > 2\sigma(I)$] | R1 = 0.0295, wR2 = 0.0702 |
| R indices (all data) | R1 = 0.0380, wR2 = 0.0723 |
| Largest diff. peak and hole | 0.723 and -0.225 e. Å ⁻³ |

Table 5.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 5 U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|--------|
| Cu(1) | 9360(1) | 8521(1) | 8501(1) | 30(1) |
| O(1) | 9105(1) | 6028(3) | 8963(1) | 43(1) |
| O(3) | 9506(2) | 8746(4) | 5595(2) | 76(1) |
| O(4) | 7881(2) | 4074(4) | 8141(1) | 65(1) |
| O(11) | 10465(1) | 8637(2) | 9094(1) | 33(1) |
| O(12) | 11294(1) | 7434(3) | 8173(1) | 43(1) |
| O(13) | 11167(1) | 9612(3) | 10403(1) | 46(1) |
| O(21) | 8218(1) | 8527(2) | 7983(1) | 36(1) |
| O(22) | 8766(1) | 7309(3) | 6910(1) | 43(1) |
| O(26) | 4941(2) | 8042(7) | 8008(1) | 123(2) |
| O(25) | 4215(1) | 7875(6) | 6961(2) | 103(1) |
| O(23) | 7070(1) | 9210(4) | 4577(1) | 63(1) |
| O(24) | 5687(1) | 8593(3) | 4550(1) | 64(1) |
| N(22) | 4902(2) | 7999(4) | 7321(1) | 55(1) |
| N(21) | 6394(2) | 8796(3) | 4886(1) | 43(1) |
| C(11) | 11208(1) | 8162(3) | 8817(1) | 30(1) |
| C(12) | 12002(1) | 8550(3) | 9318(1) | 27(1) |
| C(13) | 12828(1) | 8215(3) | 9027(1) | 33(1) |
| C(14) | 13583(2) | 8514(3) | 9474(2) | 39(1) |
| C(15) | 13509(1) | 9162(4) | 10229(1) | 39(1) |
| C(16) | 12705(1) | 9506(3) | 10527(1) | 37(1) |
| C(17) | 11943(1) | 9224(3) | 10081(1) | 31(1) |
| C(21) | 8166(1) | 7962(3) | 7284(1) | 30(1) |
| C(22) | 7268(1) | 8121(3) | 6896(1) | 29(1) |
| C(23) | 7237(1) | 8357(3) | 6098(1) | 31(1) |
| C(24) | 6418(2) | 8482(3) | 5729(1) | 31(1) |
| C(25) | 5654(2) | 8353(3) | 6104(1) | 37(1) |
| C(26) | 5714(1) | 8122(3) | 6900(1) | 36(1) |
| C(27) | 6512(1) | 8027(3) | 7303(1) | 34(1) |
| O(2) | 9719(1) | 10618(3) | 7867(1) | 66(1) |

Table 5.3 Bond lengths [\AA] and angles [$^\circ$] for compound 5

| Bond lengths | [\AA] | Bond angles | [$^\circ$] |
|--------------|------------------|--------------------|--------------|
| Cu(1)-O(2) | 1.9150(18) | H(4B)-O(4)-H(4A) | 109(5) |
| Cu(1)-O(21) | 1.9363(15) | C(11)-O(11)-Cu(1) | 123.47(12) |
| Cu(1)-O(11) | 1.9513(14) | C(17)-O(13)-H(13A) | 109.5 |
| Cu(1)-O(1) | 1.9536(18) | C(21)-O(21)-Cu(1) | 118.16(15) |
| O(1)-H(1A) | 0.8200 | O(26)-N(22)-O(25) | 122.4(3) |
| O(1)-H(1B) | 0.77(4) | O(26)-N(22)-C(26) | 118.7(2) |
| O(3)-H(3A) | 0.68(4) | O(25)-N(22)-C(26) | 118.9(2) |
| O(3)-H(3B) | 0.68(4) | O(23)-N(21)-O(24) | 124.7(2) |

Table 5.3 Bond lengths [Å] and angles [°] for compound 5 (ต่อ)

| Bond lengths | [Å] | Bond angles | [°] |
|------------------|------------|-------------------|------------|
| O(11)-C(11) | 1.285(3) | O(12)-C(11)-O(11) | 123.90(18) |
| O(12)-C(11) | 1.235(3) | O(12)-C(11)-C(12) | 119.6(2) |
| O(13)-C(17) | 1.350(3) | O(11)-C(11)-C(12) | 116.51(17) |
| O(13)-H(13A) | 0.8200 | C(13)-C(12)-C(17) | 118.62(17) |
| O(21)-C(21) | 1.272(2) | C(13)-C(12)-C(11) | 119.16(18) |
| O(22)-C(21) | 1.223(3) | C(17)-C(12)-C(11) | 122.21(19) |
| O(26)-N(22) | 1.189(3) | C(14)-C(13)-C(12) | 121.3(2) |
| O(25)-N(22) | 1.208(3) | C(14)-C(13)-H(13) | 119.4 |
| O(23)-N(21) | 1.210(3) | C(12)-C(13)-H(13) | 119.4 |
| O(24)-N(21) | 1.220(3) | C(13)-C(14)-C(15) | 119.2(2) |
| N(22)-C(26) | 1.456(3) | C(13)-C(14)-H(14) | 120.4 |
| N(21)-C(24) | 1.475(3) | C(15)-C(14)-H(14) | 120.4 |
| C(11)-C(12) | 1.494(3) | C(16)-C(15)-C(14) | 120.65(19) |
| C(12)-C(13) | 1.389(3) | C(16)-C(15)-H(15) | 119.7 |
| C(12)-C(17) | 1.407(3) | C(14)-C(15)-H(15) | 119.7 |
| C(13)-C(14) | 1.385(3) | C(15)-C(16)-C(17) | 120.6(2) |
| C(13)-H(13) | 0.9300 | C(15)-C(16)-H(16) | 119.7 |
| C(14)-C(15) | 1.390(4) | C(17)-C(16)-H(16) | 119.7 |
| C(14)-H(14) | 0.9300 | O(13)-C(17)-C(16) | 118.08(17) |
| C(15)-C(16) | 1.366(3) | O(13)-C(17)-C(12) | 122.26(16) |
| C(15)-H(15) | 0.9300 | C(16)-C(17)-C(12) | 119.7(2) |
| C(16)-C(17) | 1.391(2) | O(22)-C(21)-O(21) | 126.15(18) |
| C(16)-H(16) | 0.9300 | O(22)-C(21)-C(22) | 118.21(17) |
| C(21)-C(22) | 1.512(3) | O(21)-C(21)-C(22) | 115.64(19) |
| C(22)-C(27) | 1.370(3) | C(27)-C(22)-C(23) | 120.77(18) |
| (22)-C(23) | 1.391(3) | C(27)-C(22)-C(21) | 122.11(18) |
| C(23)-C(24) | 1.390(3) | C(23)-C(22)-C(21) | 117.12(19) |
| C(23)-H(23) | 0.9300 | C(24)-C(23)-C(22) | 118.0(2) |
| C(24)-C(25) | 1.353(3) | C(24)-C(23)-H(23) | 121.0 |
| C(25)-C(26) | 1.389(3) | C(22)-C(23)-H(23) | 121.0 |
| C(25)-H(25) | 0.9300 | C(25)-C(24)-C(23) | 123.31(19) |
| C(26)-C(27) | 1.387(3) | C(25)-C(24)-N(21) | 119.19(18) |
| C(27)-H(27) | 0.9300 | C(23)-C(24)-N(21) | 117.5(2) |
| O(2)-H(2A) | 0.8200 | C(24)-C(25)-C(26) | 116.87(18) |
| O(2)-H(2B) | 0.71(3) | C(24)-C(25)-H(25) | 121.6 |
| Bond angles | [°] | C(26)-C(25)-H(25) | 121.6 |
| O(2)-Cu(1)-O(21) | 90.01(7) | C(27)-C(26)-C(25) | 122.4(2) |
| O(2)-Cu(1)-O(11) | 90.77(7) | C(27)-C(26)-N(22) | 119.4(2) |
| O(2)-Cu(1)-O(1) | 167.03(10) | C(22)-C(27)-C(26) | 118.56(19) |
| O(21)-Cu(1)-O(1) | 90.34(7) | C(22)-C(27)-H(27) | 120.7 |
| O(11)-Cu(1)-O(1) | 89.97(7) | C(26)-C(27)-H(27) | 120.7 |
| Cu(1)-O(1)-H(1A) | 109.5 | Cu(1)-O(2)-H(2A) | 109.5 |
| Cu(1)-O(1)-H(1B) | 118(4) | Cu(1)-O(2)-H(2B) | 128(3) |
| H(1A)-O(1)-H(1B) | 105.7 | H(2A)-O(2)-H(2B) | 122.6 |

Symmetry transformations used to generate equivalent atoms:

Table 5.4 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 5. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| Cu(1) | 22(1) | 44(1) | 23(1) | 2(1) | -5(1) | -3(1) |
| O(1) | 39(1) | 48(1) | 41(1) | 8(1) | -6(1) | -6(1) |
| O(3) | 84(2) | 99(2) | 47(1) | 8(1) | 13(1) | -31(2) |
| O(4) | 55(1) | 79(2) | 60(1) | -18(1) | 14(1) | -21(1) |
| O(11) | 22(1) | 51(1) | 26(1) | 0(1) | -5(1) | -1(1) |
| O(12) | 38(1) | 58(1) | 32(1) | -14(1) | -6(1) | -1(1) |
| O(13) | 23(1) | 77(1) | 37(1) | -18(1) | -3(1) | 2(1) |
| O(21) | 26(1) | 55(1) | 26(1) | -4(1) | -5(1) | -2(1) |
| O(22) | 28(1) | 64(1) | 36(1) | -5(1) | -3(1) | 11(1) |
| O(26) | 49(1) | 275(5) | 46(1) | 16(2) | 15(1) | 9(2) |
| O(25) | 25(1) | 203(3) | 82(2) | 3(2) | 1(1) | -7(2) |
| O(23) | 60(1) | 91(2) | 37(1) | 14(1) | 4(1) | 1(1) |
| O(24) | 57(1) | 90(2) | 42(1) | -1(1) | -26(1) | 14(1) |
| N(22) | 29(1) | 84(2) | 54(1) | 6(1) | 8(1) | 4(1) |
| N(21) | 47(1) | 50(1) | 31(1) | 1(1) | -8(1) | 9(1) |
| C(11) | 26(1) | 34(1) | 29(1) | 2(1) | -5(1) | -2(1) |
| C(12) | 23(1) | 31(1) | 26(1) | 0(1) | -4(1) | 2(1) |
| C(13) | 28(1) | 38(1) | 32(1) | -3(1) | 0(1) | 2(1) |
| C(14) | 23(1) | 46(1) | 47(1) | -1(1) | -1(1) | 2(1) |
| C(15) | 25(1) | 47(1) | 44(1) | -1(1) | -9(1) | -1(1) |
| C(16) | 28(1) | 49(1) | 32(1) | -5(1) | -7(1) | 0(1) |
| C(17) | 24(1) | 39(1) | 29(1) | -3(1) | -2(1) | 1(1) |
| C(21) | 24(1) | 39(1) | 27(1) | 1(1) | -4(1) | -1(1) |
| C(22) | 24(1) | 35(1) | 29(1) | -3(1) | -5(1) | 1(1) |
| C(23) | 26(1) | 37(1) | 29(1) | -1(1) | -2(1) | 1(1) |
| C(24) | 31(1) | 36(1) | 27(1) | 0(1) | -6(1) | 3(1) |
| C(25) | 26(1) | 43(1) | 40(1) | 1(1) | -10(1) | 2(1) |
| C(26) | 24(1) | 47(1) | 37(1) | -1(1) | 1(1) | 2(1) |
| C(27) | 27(1) | 49(1) | 27(1) | -2(1) | -2(1) | 3(1) |
| O(2) | 41(1) | 85(2) | 70(1) | 48(1) | -30(1) | -26(1) |

Table 5.5 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound 5

| | x | y | z | U(eq) |
|--------|----------|-----------|----------|---------|
| H(1A) | 8777 | 5416 | 8672 | 64 |
| H(13A) | 10766 | 9281 | 10107 | 69 |
| H(13) | 12875 | 7781 | 8521 | 39 |
| H(14) | 14132 | 8285 | 9272 | 46 |
| H(15) | 14013 | 9362 | 10533 | 47 |
| H(16) | 12666 | 9934 | 11034 | 44 |
| H(23) | 7749 | 8429 | 5820 | 37 |
| H(25) | 5115 | 8417 | 5842 | 44 |
| H(27) | 6533 | 7903 | 7838 | 41 |
| H(2A) | 10226 | 10915 | 7983 | 99 |
| H(3A) | 9290(20) | 8230(50) | 5870(20) | 55(11) |
| H(3B) | 9210(30) | 8570(60) | 5300(30) | 100(20) |
| H(2B) | 9470(20) | 11090(50) | 7571(19) | 57(10) |
| H(1B) | 9490(30) | 5350(70) | 9060(30) | 111(16) |
| H(4B) | 7490(40) | 3650(80) | 8270(30) | 140(20) |
| H(4A) | 8060(20) | 3450(40) | 7750(20) | 54(9) |

Table 5.6 Torsion angles [$^\circ$] for compound 5

| Torsion angles | [$^\circ$] | Torsion angles | [$^\circ$] |
|-------------------------|--------------|-------------------------|--------------|
| O(2)-Cu(1)-O(11)-C(11) | -69.33(17) | O(22)-C(21)-C(22)-C(27) | 151.6(2) |
| O(21)-Cu(1)-O(11)-C(11) | -168.7(7) | O(21)-C(21)-C(22)-C(27) | -28.1(3) |
| O(1)-Cu(1)-O(11)-C(11) | 97.73(16) | O(22)-C(21)-C(22)-C(23) | -28.0(3) |
| O(2)-Cu(1)-O(21)-C(21) | 70.21(17) | O(21)-C(21)-C(22)-C(23) | 152.3(2) |
| O(11)-Cu(1)-O(21)-C(21) | 169.6(7) | C(27)-C(22)-C(23)-C(24) | -0.4(3) |
| O(1)-Cu(1)-O(21)-C(21) | -96.83(16) | C(21)-C(22)-C(23)-C(24) | 179.21(18) |
| Cu(1)-O(11)-C(11)-O(12) | -6.3(3) | C(22)-C(23)-C(24)-C(25) | -1.1(3) |
| Cu(1)-O(11)-C(11)-C(12) | 173.16(13) | C(22)-C(23)-C(24)-N(21) | 178.04(18) |
| O(12)-C(11)-C(12)-C(13) | 4.7(3) | O(23)-N(21)-C(24)-C(25) | 168.5(2) |
| O(11)-C(11)-C(12)-C(13) | -174.77(18) | O(24)-N(21)-C(24)-C(25) | -12.3(3) |
| O(12)-C(11)-C(12)-C(17) | -174.51(19) | O(23)-N(21)-C(24)-C(23) | -10.7(3) |
| O(11)-C(11)-C(12)-C(17) | 6.0(3) | O(24)-N(21)-C(24)-C(23) | 168.5(2) |
| C(17)-C(12)-C(13)-C(14) | 0.6(3) | C(23)-C(24)-C(25)-C(26) | 1.2(3) |
| C(11)-C(12)-C(13)-C(14) | -178.6(2) | N(21)-C(24)-C(25)-C(26) | -177.92(19) |
| C(12)-C(13)-C(14)-C(15) | 0.0(3) | C(24)-C(25)-C(26)-C(27) | 0.1(3) |
| C(13)-C(14)-C(15)-C(16) | -0.2(4) | C(24)-C(25)-C(26)-N(22) | 179.4(2) |
| C(14)-C(15)-C(16)-C(17) | -0.3(4) | O(26)-N(22)-C(26)-C(27) | 8.5(4) |
| C(15)-C(16)-C(17)-O(13) | -179.1(2) | O(25)-N(22)-C(26)-C(27) | -172.1(3) |
| C(15)-C(16)-C(17)-C(12) | 0.9(3) | O(26)-N(22)-C(26)-C(25) | -170.8(3) |
| C(13)-C(12)-C(17)-O(13) | 178.9(2) | O(25)-N(22)-C(26)-C(25) | 8.6(4) |
| C(13)-C(12)-C(17)-C(16) | -1.1(3) | C(21)-C(22)-C(27)-C(26) | -177.9(2) |
| C(11)-C(12)-C(17)-C(16) | 178.16(19) | C(25)-C(26)-C(27)-C(22) | -1.6(3) |
| Cu(1)-O(21)-C(21)-O(22) | 4.1(3) | N(22)-C(26)-C(27)-C(22) | 179.2(2) |
| Cu(1)-O(21)-C(21)-O(22) | 4.1(3) | N(22)-C(26)-C(27)-C(22) | 179.2(2) |

Symmetry transformations used to generate equivalent atoms:

Table 5.7 Hydrogen bonds for mono [\AA and $^\circ$].

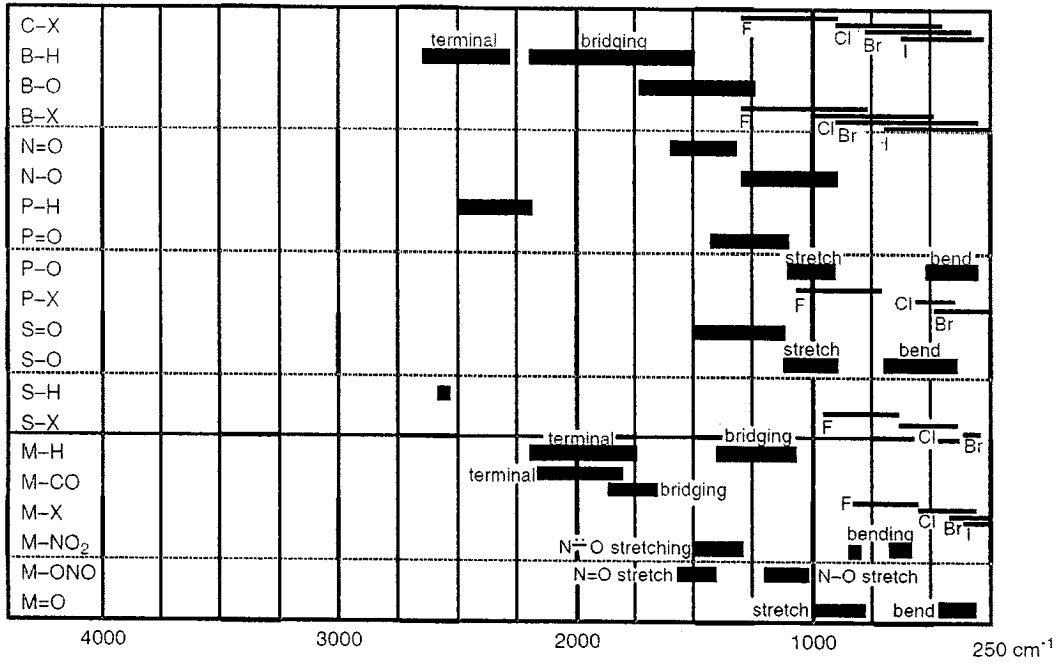
| D-H | d(D-H) | d(H..A) | \angle DHA | d(D..A) | A |
|----------|--------|---------|--------------|---------|-----------------------------|
| O1-H1A | 0.820 | 1.874 | 169.88 | 2.685 | O4 |
| O13-H13A | 0.820 | 1.856 | 144.99 | 2.571 | O11 |
| O2-H2A | 0.820 | 1.823 | 161.03 | 2.612 | O22 [-x+2, y+1/2, -z+3/2] |
| O3-H3A | 0.685 | 2.097 | 162.61 | 2.758 | O22 |
| O3-H3B | 0.682 | 2.334 | 138.01 | 2.878 | O1 [x, -y+3/2, z-1/2] |
| O2-H2B | 0.707 | 1.954 | 174.54 | 2.659 | O12 [-x+2, y+1/2, -z+3/2] |
| O1-H1B | 0.766 | 1.975 | 175.02 | 2.739 | O3 [-x+2, y-1/2, -z+3/2] |
| O4-H4A | 0.855 | 2.028 | 166.90 | 2.868 | O12 [-x+2, y-1/2, -z+3/2] |

ภาคผนวก 3 ข้อมูลอินฟราเรดสเปกโทรโฟโตมิเตอร์

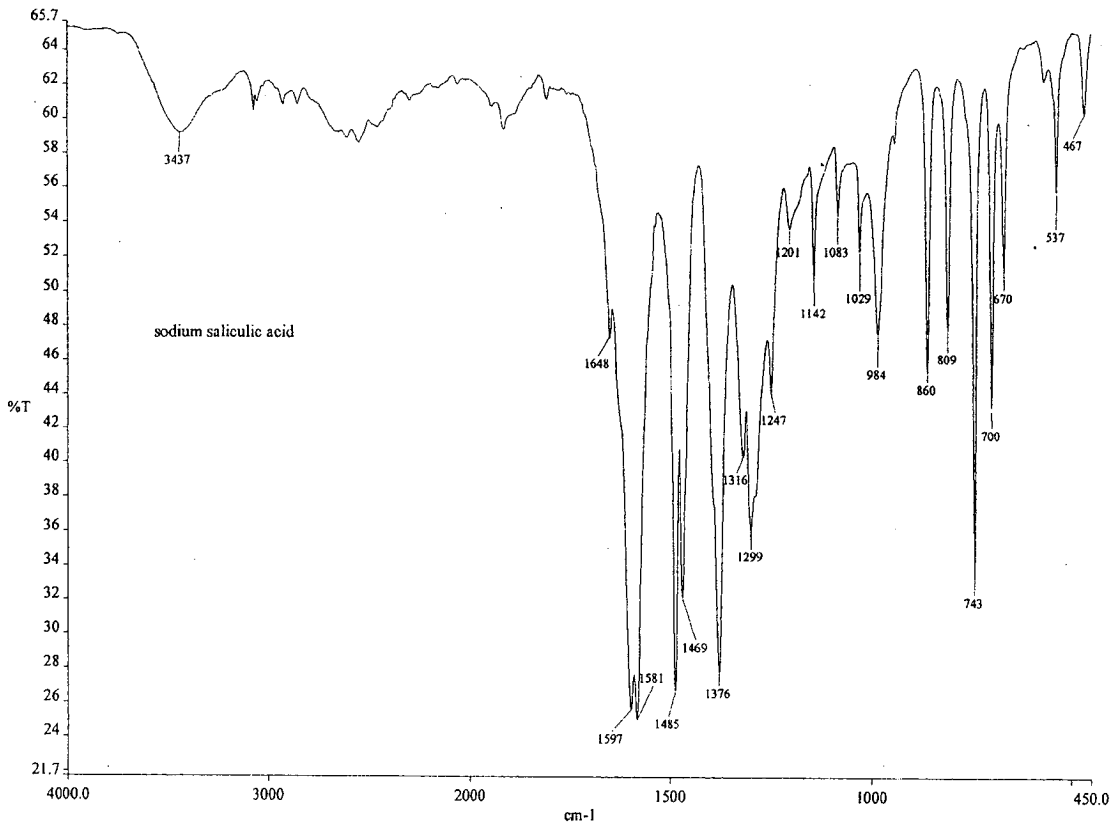
ภาคผนวก 3.1 สเปกตรัมอินฟราเรดของสารประกอบ 1-5 และที่เกี่ยวข้องอ้างอิงจาก R.M. Silverstein

| 1 | 2 | 3 | CuCl ₂ . 2H ₂ O | 4 | 5 | Frequency, cm ⁻¹ | Bond | Functional group |
|-------------|-------------|------------------------|--|-------------|---------------------|--------------------------------|-------------------------------|----------------------|
| | 3748(s) | >3447(s) | 3367(s) | >3360(s) | >3425(s) | 3640-3610 (s, sh) | O-H stretch, free hydroxyl | alcohols, phenols |
| | 3455(m) | 3447(m) | | 3360(m) | 3425(m) | 3300-2500 (m) | O-H stretch | carboxylic acids |
| 3093(s) | 3097(s) | 3120(s) 3062(m) | | 3102(s) | 3093(s) 2928(ms) | 3100-3000 (s) | C-H stretch | aromatics |
| 1704(s) | 1734(s) | 1679(s) | 1602(s) | 1618(s) | 1624(s) | 1760-1665 (s) | C=O stretch | carboxylic acids |
| 1631(m) | 1629(m) | 1613(m) | | 1593(m) | 1577(m) | 1600-1585 (m) | C-C stretch (in-ring) | aromatics |
| 1547(s) | 1545(s) | 1570(s) | | 1542 (s) | 1542 (s) | 1550-1475 (s) | N-O asymmetric stretch | nitro compounds |
| 1471 (m) | 1469(m) | 1453(m) 1407 (m) | | 1467(m) | 1457 (m) | 1500-1400 (m) | C-C stretch (in-ring) | aromatics |
| 1348(m) | 1347 (m) | 1391 (m) | | 1345 (m) | 1346 (m) | 1360-1290 (m) | N-O symmetric stretch | nitro compounds |
| 1286(s) | 1278 (s) | 1281 (m) | | 1251 (s) | (s) | 1320-1210 (s) | C-O stretch | carboxylic acids |
| 923 (m) | 923(m) | 834(m) | | 919 (m) | 916 (m) | 950-910 (m) | O-H bend | carboxylic acids |
| 697 (s) | 665 (s) | 684(s) | | 697 (s) | 674 (s) | 900-675 (s) | C-H "oop" | aromatics |
| 722 (m) | 723 (m) | 726 (m) 712 (m) | | 730 (m) | 729 (m) | 725-720 (m) | C-H rock | alkanes |
| | | 504(m) | 566 (m) | 526 (m) | 535 (m) | 590-520 (m) | Cu-O stretch | Metal-O |

ภาคผนวก 3.2 อินฟราเรดสเปกตรัมจาก A.K. Brisdon

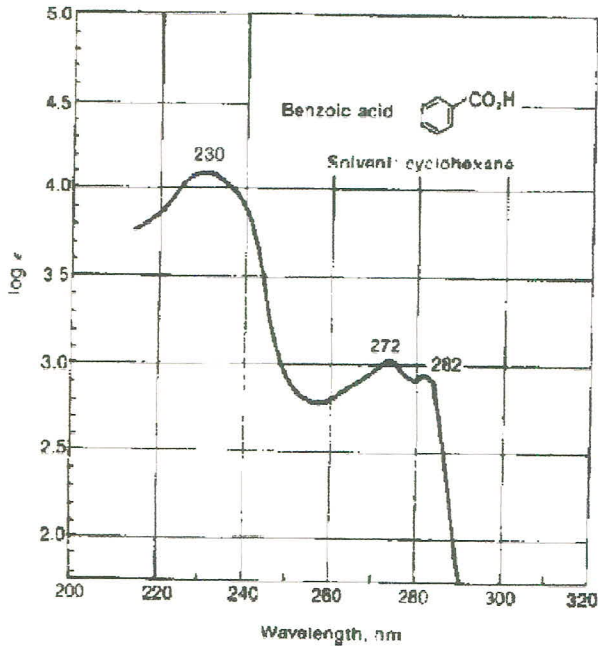


ภาคผนวก 3.3 สเปกตรัมอินฟราเรดของโซเดียมซาลิไซเลต



ภาคผนวก 4 ข้อมูลอัตราไวโอเลต-วิสิเบิล สเปกโทรโฟโตมิเตอร์

ภาคผนวก 4.1 สเปกตรัมอัตราไวโอเลต-วิสิเบิล ของกรดเบนโซอิกในไซโคลเฮกเซน



| | |
|--|-----------------------|
| $\lambda_{\text{max}} = 230\text{nm}:$ | $\log \epsilon = 4.2$ |
| 272 | 3.1 |
| 282 | 2.9 |

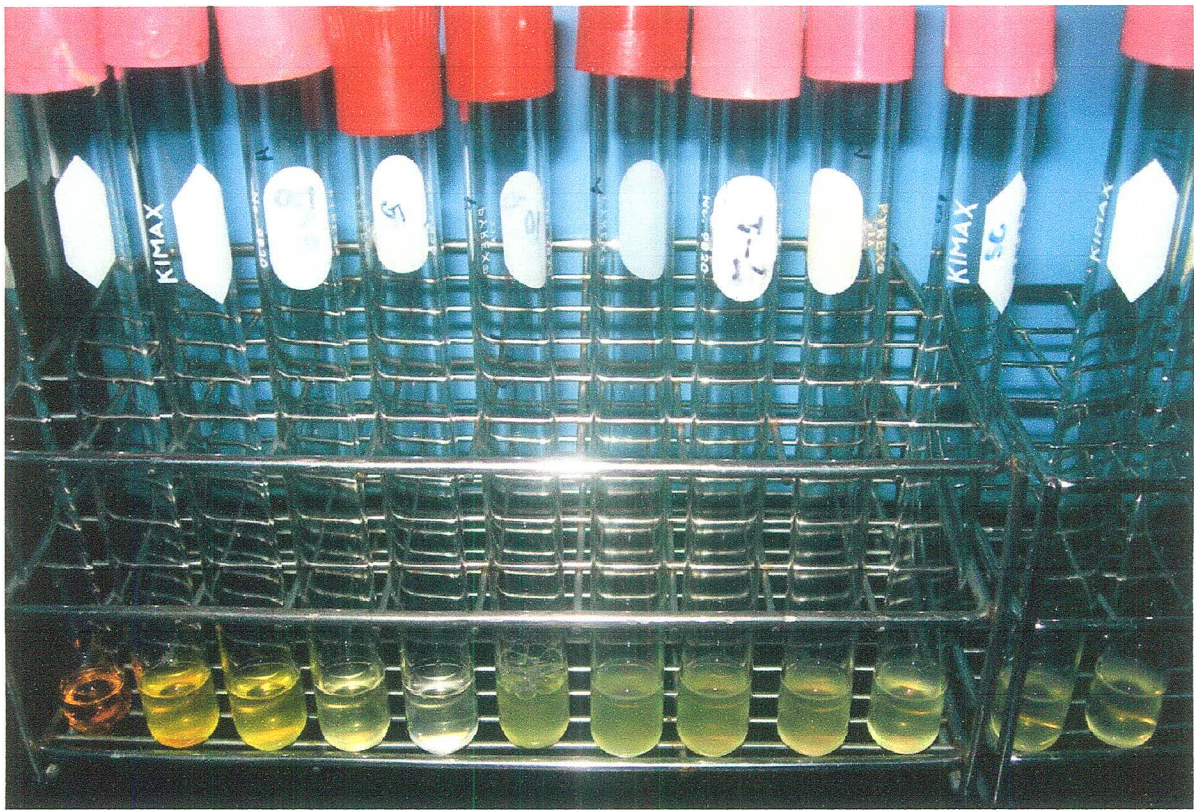
แหล่งที่มา : BUCHI Labortechnik AG หรือ www.buchi.com

ภาคผนวก 5 ข้อมูลศึกษาฤทธิ์ต้านจุลชีพ

ภาคผนวก 5.1 การหาค่า MIC ในการยับยั้งเชื้อ *E.coli* ของสารประกอบ 3



ภาพผนวก 5.2 การหาค่า MIC ในการยับยั้งเชื้อ *P.aeruginosa* ของสารประกอบ 3



ภาพผนวก 5.3 การหาค่า MIC ในการยับยั้งเชื้อ *S. aureus* ของสารประกอบ 3

