|  |  |  |
| --- | --- | --- |
| Compound  | [Cu(phen)2(CH3COO)](ClO4).2H2O | [Cu(bipy)2(CH3COO)](ClO4).H­2O |
| CCDC deposit no | 1418811  |  1418812 |
| Color/Shape | Bluish-green/block |  Blue/rod |
| Chemical formula | C26H23ClCuN4O8 | C22 H21Cl Cu N4 O7 |
| Formula weight | 618.47 | 552.42 |
| Temperature, K | 100(2) | 100(2) |
| Wavelength | 0.71073 Å | 0.71073 Å |
| Crystal system | Monoclinic | Triclinc |
| Space group | P n | P-1 |
| Unit cell dimensions | a = 9.3682(6)Å | a = 8.2822(4) Å |
|  | b = 8.3029(5) Å | b = 9.4748(4) Å |
|  | c = 16.8784(10) Å | c = 14.7992(6) Å |
|  |  β = 103.3014(18)° | α = 78.729(2)° |
|  |  | β = 82.881(2)° |
|  |  | γ = 85.092(2)° |
| Volume | 1277.64(14) Å3 | 1127.90(9) Å3 |
| Z | 2 | 2 |
| Density(calculated) | 1.608 Mg/m3 | 1.627Mg/m3 |
| Absorption coefficient, mm-1 | 1.019 | 1.140 |
| Θ range for data collection,deg | 2.292 – 30.570 | 2.20-30.58 |
| Reflections method | 9896 | 58024 |
| Independent reflections | 6312[R(int) = 0.0196] | 6914[R(int) = 0.0421] |
| Data/restraints/parameters | 6312/8/379 | 6914/68/339 |
| Goodness-of fit on F2 | 1.070 | 1.083 |
| Final R indices [I>2sigma(I)]  | R1 = 0.0325, wR2 = 0.0772 | R1 = 0.0357, wR2 = 0.0776 |
| R indices (all data) | R1 = 0.0377, wR2 = 0.0802 | R1 = 0.0451, wR2 = 0.0814 |
| Absolute structure parameter 26 | 0.521(12) | - |

Table I. Crystal Data and Structural Refinement for [Cu(phen)2(CH3COO)](ClO4).2H2O and [Cu(bipy)2(CH3COO)](ClO4).H­2O