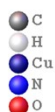
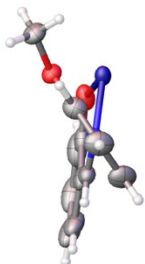


File Edit View Structure Mode Tools Model Select Help



```
***** After 10 CYCLES ***  
R1: 0.0433 for 2842 reflections I >= 2σ(I)  
R1 (all): 0.0587 for 3520 reflections  
wR2: 0.1292, GoodF: 1.0617  
Diff: max=1.08, min=-0.58  
Shifts: xyz: 0.0000 for H12, U: 0.0000 for Cu1, Max/esd = 0.0008 for H12, also  
***** 22 Constraints | 0 Restraints | 159 Parameters *****  
no is conflicting information in the sources of metadata  
uding report request
```

**Final\_3\_solve** *1a3 d*  
C<sub>20</sub>H<sub>21</sub>CuN<sub>2</sub>O<sub>4</sub>  
a = 31.0995(7) Å α = 90° Z = 4 R<sub>1</sub> = 4.33 %  
b = 31.0995(7) Å β = 90° Z' = 0.5  
c = 31.0995(7) Å γ = 90° V = 30078.8(12) Å<sup>3</sup> WR<sub>2</sub> = 12.92 %  
S min (H<sub>2</sub>O) 0.72 min 59.5 max 7.94% complete 100%  
Shift 0.001 Max Peak 1.1 Min Peak -0.6 GoodF 1.062

Home Work View Tools Info  
Solve Refine Draw Report

Final\_3\_solve Image no image Make Report  
Style default.cas Begin with default.htm End with templates/foe  
Table label style: As in CIF

Collection  
Crystal  
Crystal Image

Diffraction  
Absorption Correction  
Publication  
Citations  
Reference  
Source Files

Edit CIF info Merge CIF HKLRES Leave as is  
R1C1 CheckCIF pdf CCDC Request CCDC Number  
Merge CIF: manual Add local | default CIF  
 Merge metaCIF items even if marked for skipping

Toolbox Work  
Labels Labels OFF/ON  
C H N O ... Add H  
SH H C F I O Z= 0.5