anglefinder

version 0.11 based on pymatgen version 2019.9.16

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Search criteria:

d atom: Cu
ligand: O
maximal distance between a d atom and a ligand: 2.100
maximal distance between d atoms: 3.100
minimal number of common ligands: 2
minimal d-lingand-d angle: 93.60
maximal d-lingand-d angle: 94.00
```

compound	cif file	d-ligand-d angles
$Cu_2BH_5O_6$	054883.cif	**93.98** 97.17 97.37 99.59
$Sr_{3.72}Nd_{0.28}Cu_4O_8$	075842.cif	**93.87**
$Na_2Cu_5(W_2O_{13})_6$	420587.cif	**93.99**
$Al_{5.08}Fe_{2.92}Cu_8As_8O_{48}$	158357.cif	91.80 92.43 **93.91** 95.29
$Rb_2V_6CdCu_9O_{26}$	406788.cif	93.45 **93.99** 96.78 100.80
$CuSiO_3$	089669.cif	**93.73**
$V_4Cu_9(ClO_9)_2$	190682.cif	88.96 91.92 92.68 93.36 **93.63** **93.78** 95.31
Cu_2SO_5	061513.cif	**93.63**
$BaV_2(CuO_4)_2$	033804.cif	**93.67**
$Al_{5.08}Fe_{2.92}Cu_8As_8O_{48}$	005030.cif	91.80 92.43 **93.91** 95.29
$Na_5(CuO_2)_3$	185337.cif	93.12 **93.66** 94.12 94.38 95.67 97.20
$K_3FeCu_7(AsO_5)_4$	257353.cif	**93.98** 96.59 96.82 98.49
$Y_2Cu_2O_5$	202877.cif	92.54 **93.65**
$V_2(CuO_2)_5$	002557.cif	91.91 92.39 **93.68** 96.20 99.42
Li_2CuO_2	067151.cif	**93.74**
$Cu_3NiP_2O_9$	425977.cif	**93.76** 100.16

compound	cif file	d-ligand-d angles
$Ca_2Cu_2Si(WO_7)_8$	249629.cif	**93.81** 99.29
Li_2CuO_2	067204.cif	**93.97**
$Ca_{9.6}Pr_{6.4}Cu_{20}O_{40}$	099569.cif	86.87 87.45 89.89 92.33 **93.87 93.89**
		93.93 96.13 98.37 98.62
$Cu_4Se_3O_{10}$	060654.cif	92.22 92.52 **93.76 93.93** 99.76 100.36
		100.47 101.74 101.78 102.20 103.04 105.53
$Ho_2Cu_2O_5$	079428.cif	92.14 **93.78**
$K_2Cu_5H_8(Cl_4O_3)_2$	055096.cif	**93.78** 95.60
$V_2Cu_5(HO_3)_4$	054831.cif	**93.66** 99.84 101.78
$KCu_4(PO_4)_3$	065123.cif	**93.93** 97.25
$K_4Cu_4Si_2W_{16}O_{81}$	159481.cif	**93.89** 99.59
Cu_3AsO_7	068456.cif	**93.61** 99.93
$NaCu_5Se_2Cl_3O_8$	264483.cif	90.79 **93.60** 95.87 101.41
$Cu_5(PO_6)_2$	010418.cif	**93.64** 95.45 96.68
Cu_2CO_5	262802.cif	**93.68** 98.12
$Li_{3.6}V_4Cu_{3.996}O_{16}$	072847.cif	**93.84**
$Ca_{10}Pr_4Cu_{24}O_{41}$	099568.cif	68.82 86.85 87.53 88.00 89.14 89.80
		90.24 90.39 90.95 **93.76**
$Ca_4Cu_4As_{1.8}P_{2.2}O_{20}$	247659.cif	**93.96** 95.04
$Ca_{9.6}Pr_{6.4}Cu_{20}O_{40}$	054900.cif	86.87 87.45 89.89 92.33 **93.87 93.89**
		93.93 96.13 98.37 98.62
$Cu_4As_2O_9$	239832.cif	18.47 18.70 19.13 92.81 **93.69 93.72**
		94.04 95.23 98.24 100.47
$Cu_{27}P_6H_{163}W_{60.5}C_{42}N_{38}O_{270}$	238771.cif	**93.91** 94.28 94.35 96.93 98.16 100.02
Li_2CuO_2	202996.cif	**93.89**
$CuMoO_4$	190443.cif	**93.79** 96.66
$Cu_3NiP_2O_9$	380494.cif	**93.75** 100.17

compound	cif file	d-ligand-d angles
$Cu_{3.788}H_8Pb_{3.868}Se_{1.7}S_{2.3}O_{22}$	182701.cif	92.70 **93.77** 94.60 95.48
$Cu_9Se_4(Cl_3O_7)_2$	091804.cif	**93.77** 94.57 97.25 98.81
$Cu_{12}Bi_2As_6O_{37.9998}$	050062.cif	**93.77** 97.49 100.60 101.98
$Tm_2Cu_2O_5$	069329.cif	92.30 **93.95**
$Sr_{11.7}Ca_{27.7}Nd_{14.64}Y_{5.36}Cu_{92.6}O_{164}$	039941.cif	59.45 70.27 74.63 78.41 79.82 80.53
		85.04 85.74 87.52 87.99 88.37 89.02
		89.10 89.26 89.69 90.05 91.35 **93.82**
		97.29 97.83 110.10 114.20
Li_2CuO_2	067205.cif	**93.96**
$Cu_3H_{30}C_{10}S_3N_4O_{15}$	248823.cif	**93.93**
$Na_5(CuO_2)_3$	422413.cif	93.13 **93.68** 94.13 94.43 95.68 97.22
$ZnCu_2PO_8$	188025.cif	**93.63** 97.10 98.08
$MnCu_4H_{14}(SO_9)_2$	030797.cif	**93.91** 102.04
Cu_3AsO_7	087869.cif	**93.74** 96.38 96.47 97.04
$Cu_2Pb_2Se_2O_{11}$	068172.cif	92.43 92.64 **93.71** 94.66

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Searching in a pool of 719 cif files.

Warnings:

Structure 158337.cif is corrupt.
Structure 158336.cif is corrupt.
Structure 071825.cif is corrupt.
Structure 068662.cif is corrupt.
Structure 085128.cif is corrupt.
Structure 158338.cif is corrupt.
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