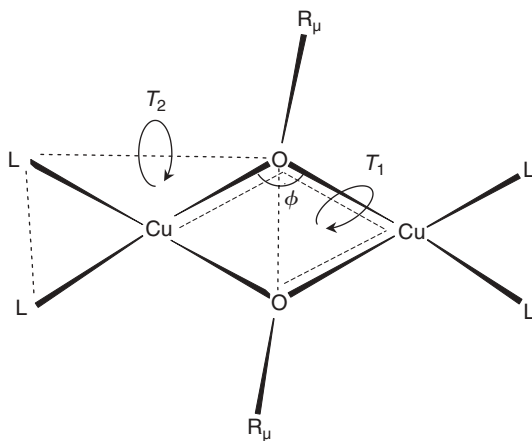


Table 1. Structural data for CuO₂Cu compoundsB₁–B₄: Cu–O bond lengths. ϕ_1, ϕ_2 : Cu–O–Cu' bond angles. ϕ : average Cu–O–Cu' bond angle. r : Cu···Cu distance. T_1 : O–Cu–O–Cu torsion. T_2 : L–L–O–O torsion. nL: number of ligands on each copper. CuL: ligand atoms on copper.^A R _{μ} : atoms attached to bridging oxygen atom.^ACL: whether the CuO₂Cu moiety is part of a cluster. $2J$: isotropic exchange-coupling constant

| Structure ^B | B ₁ | B ₂ | B ₃ | B ₄ | ϕ_1 | ϕ_2 | ϕ | r | T_1 | T_2 | nL | CuL | R _{μ} | CL | $2J$ | Reference |
|------------------------|----------------|----------------|----------------|----------------|----------|----------|--------|-------|-------|-------|-----|---------|-------------------------------|-----|--------|-----------|
| 1. | 1.926 | 1.909 | 1.909 | 1.926 | 103.4 | 103.4 | 103.4 | 3.009 | 0.0 | 10.0 | 4 | NO | C | | -800 | [1] |
| 2. | 1.943 | 1.948 | 1.948 | 1.943 | 103.5 | 103.5 | 103.5 | 3.056 | 0.0 | 3.3 | 5 | NOO | C | | -740 | [2] |
| 3. | 1.939 | 1.927 | 1.927 | 1.939 | 101.6 | 101.6 | 101.6 | 2.996 | 0.0 | 9.9 | 5 | NSCI | C | | -400 | [3] |
| 4. | 1.938 | 1.931 | 1.931 | 1.938 | 102.5 | 102.5 | 102.5 | 3.018 | 0.0 | 15.1 | 5 | NSCI | C | | -425 | [3] |
| 5. | 1.944 | 1.941 | 1.941 | 1.944 | 101.6 | 101.6 | 101.6 | 3.010 | 0.0 | 15.9 | 5 | NSCI | C | | -215 | [4] |
| 6. | 1.932 | 1.928 | 1.928 | 1.932 | 104.2 | 104.2 | 104.2 | 3.046 | 0.0 | 6.3 | 5 | NSCI | C | | -745 | [3] |
| 7. | 1.93 | 1.939 | 1.939 | 1.93 | 101.2 | 101.2 | 101.2 | 2.991 | 0.0 | 13.8 | 5 | NSCI | C | | -340 | [3] |
| 8. | 1.899 | 1.901 | 1.901 | 1.899 | 103.1 | 103.1 | 103.1 | 2.975 | 0.0 | 8.3 | 4 | OO | C | | -373.7 | [5] |
| 9. | 2.002 | 1.94 | 1.927 | 1.94 | 102.0 | 103.8 | 102.9 | 3.053 | -3.3 | 16.0 | 5 | NNN | C/H | | -420 | [6] |
| 10. | 1.903 | 1.949 | 1.905 | 1.956 | 100.5 | 97.1 | 98.8 | 2.927 | 12.0 | 3.4 | 4 | NN | C/H | | -142 | [7] |
| 11. | 1.928 | 1.93 | 1.93 | 1.928 | 102.2 | 102.2 | 102.2 | 3.002 | 0.0 | 14.8 | 5 | NBrS | C | | -735 | [8] |
| 12. | 1.923 | 1.92 | 1.92 | 1.923 | 95.6 | 95.6 | 95.6 | 2.848 | 0.0 | 3.5 | 4 | NN | H | | 172 | [9] |
| 13. | 1.961 | 1.941 | 1.941 | 1.961 | 101.4 | 101.4 | 101.4 | 3.019 | 0.0 | 41.7 | 4 | NBr | C | | -440 | [10] |
| 14. | 1.928 | 1.946 | 1.946 | 1.928 | 103.6 | 103.6 | 103.6 | 3.045 | 0.0 | 0.0 | 4 | NO | C | | -850 | [11] |
| 15. | 1.899 | 1.91 | 1.91 | 1.899 | 103.6 | 103.6 | 103.6 | 2.994 | 0.0 | 6.5 | 4 | NO | C | | -920 | [12] |
| 16. | 1.91 | 1.909 | 1.909 | 1.91 | 102.1 | 102.1 | 102.1 | 2.970 | 0.0 | 11.9 | 4 | OO | C | | -647 | [13] |
| 17. | 1.923 | 1.9 | 1.9 | 1.923 | 103.5 | 103.5 | 103.5 | 3.002 | 0.0 | 5.4 | 4 | NN | C | | -1015 | [14] |
| 18. | 1.923 | 1.966 | 1.966 | 1.923 | 103.3 | | 103.3 | 3.050 | | | 4 | NCl | C | | -480 | [15] |
| 19. | 1.983 | 1.929 | 1.929 | 1.983 | 103.4 | 103.4 | 103.4 | 3.069 | 0.0 | 46.8 | 4 | NCl | C | | -290 | [16] |
| 20. | 1.938 | 1.962 | 1.973 | 1.978 | 104.4 | 102.5 | 103.5 | 3.081 | -1.5 | 1.6 | 5 | NNN | C/H | | -600 | [17] |
| 21. | 1.933 | 1.917 | 1.917 | 1.933 | 103.6 | 103.6 | 103.6 | 3.026 | 0.0 | 15.8 | 4 | NO | C | | -800 | [1] |
| 22. | 1.947 | 1.936 | 1.936 | 1.947 | 98.4 | 98.4 | 98.4 | 2.939 | 0.0 | 4.2 | 4 | NN | H | | -205 | [18] |
| 23. | 2.405 | 2.003 | 1.877 | 1.907 | 89.3 | 101.7 | 95.5 | 3.033 | -25.9 | | 4/6 | NN/OOOO | C | | -44.8 | [19] |
| 24. | 2.336 | 2.024 | 1.875 | 1.922 | 95.2 | 104.7 | 100.0 | 3.125 | 7.8 | 4.1 | 4/6 | NN/OOOO | C | | -20.4 | [20] |
| 25. | 1.918 | 1.918 | 1.918 | 1.918 | 96.9 | 96.9 | 96.9 | 2.871 | 0.0 | 4.4 | 4 | NN | H | | 93 | [21] |
| 26. | 1.898 | 1.916 | 1.980 | 2.001 | 104.7 | 98.7 | 101.7 | 3.021 | 3.05 | 10.0 | 5 | NNO | C/H | | -569 | [22] |
| 27. | 1.955 | 2.49 | 2.49 | 1.955 | 95.3 | 95.3 | 95.3 | 3.306 | 0.0 | 58.2 | 5 | NNO | C | | -0.5 | [23] |
| 28. | 1.926 | 1.955 | 1.955 | 1.926 | 96.1 | 96.1 | 96.1 | 2.887 | 0.0 | 12.5 | 5 | NNO | C | | -430 | [24] |
| 29. | 1.957 | 1.964 | 1.964 | 1.957 | 98.3 | 98.3 | 98.3 | 2.966 | 0.0 | 9.0 | 5 | NNO | C | | -72 | [24] |
| 30. | 1.929 | 1.913 | 1.913 | 1.929 | 102.4 | 102.4 | 102.4 | 2.995 | 0.0 | 3.9 | 5 | NNO | C | | -380 | [24] |
| 31. | 2.35 | 1.968 | 1.968 | 2.35 | 100.0 | 100.0 | 100.0 | 3.316 | 0.0 | 63 | 5 | NNO | C | | 4.3 | [25] |
| 32. | 2.005 | 1.905 | 1.963 | 1.906 | 99.1 | 104.9 | 102.0 | 3.020 | -0.9 | 38 | 5 | NSS | C/H | | -600 | [26] |
| 33. | 2.533 | 2.000 | 1.923 | 2.377 | 95.3 | 98.2 | 96.8 | 3.319 | 29.6 | 20 | 5 | NOO | C | yes | -9.7 | [27] |
| 34. | 2.027 | 1.904 | 2.000 | 2.419 | 104.9 | 94.5 | 99.7 | 3.192 | -9.0 | 0.5 | 5 | NNO | C/H | yes | -12 | [28] |
| 35. | 2.577 | 1.976 | 1.976 | 2.577 | 96.1 | 96.1 | 96.1 | 3.409 | 0.0 | 1.9 | 6 | NNOO | C | | -1.51 | [29] |
| 36. | 2.665 | 2.003 | 2.003 | 2.665 | 96.3 | 96.3 | 96.3 | 3.506 | 0.0 | 4.2 | 6 | NNOO | C | | -1.84 | [29] |
| 37. | 1.96 | 2.498 | 2.498 | 1.96 | 98.1 | 98.1 | 98.1 | 3.384 | 0.0 | 57 | 5 | NNO | C | | -2.31 | [30] |
| 38. | 1.938 | 1.919 | 1.932 | 1.916 | 99.2 | 100.4 | 99.8 | 2.947 | 12.4 | 6.5 | 5 | NNO | C/H | | -364 | [31] |
| 39. | 1.982 | 1.93 | 1.927 | 1.913 | 99.9 | 102.2 | 101.1 | 2.992 | -7.7 | 4.4 | 4/5 | NN/NNO | C/H | | -499 | [31] |
| 40. | 1.952 | 1.919 | 1.919 | 1.952 | 99.1 | 99.1 | 99.1 | 2.946 | 0.0 | 9.3 | 5 | NCIS | C | | -350 | [32] |
| 41. | 1.945 | 1.932 | 1.938 | 1.917 | 98.1 | 99.3 | 98.7 | 2.932 | -2.7 | 8.2 | 4 | NN | C | | -367 | [33] |
| 42. | 1.954 | 1.952 | 1.956 | 1.928 | 98.3 | 99.3 | 98.8 | 2.957 | 1.8 | 14 | 4 | NN | C/H | | -493 | [34] |
| 43. | 1.924 | 1.898 | 1.898 | 1.924 | 104.1 | 104.1 | 104.1 | 3.013 | 0.0 | 0.1 | 4 | NO | C | | -600 | [35] |
| 44. | 1.926 | 1.896 | 1.896 | 1.926 | 103.2 | 103.2 | 103.2 | 2.995 | 0.0 | 7.6 | 4 | NO | C | | -600 | [35] |

(continued)

Table 1. (continued)

| Structure ^B | B ₁ | B ₂ | B ₃ | B ₄ | ϕ_1 | ϕ_2 | ϕ | r | T_1 | T_2 | nL | CuL | R _{μ} | CL | 2J | Reference |
|------------------------|----------------|----------------|----------------|----------------|----------|----------|--------|-------|-------|-------|-----|----------|-------------------------------|-----|--------|-----------|
| 45. | 2.525 | 1.918 | 1.884 | 1.961 | 88.9 | 107.2 | 98.0 | 3.121 | 12.1 | 40 | 5 | NNO | C | | -22 | [36] |
| 46. | 1.924 | 1.961 | 1.961 | 1.924 | 103.3 | 103.3 | 103.3 | 3.047 | 0.0 | 43.6 | 4 | NCI | C | | -360 | [37] |
| 47. | 1.968 | 1.999 | 1.923 | 1.962 | 98.7 | 96.4 | 97.5 | 2.952 | -6.6 | 7.6 | 4 | NN | C | | 43 | [38] |
| 48. | 1.934 | 1.965 | 1.965 | 1.934 | 103.1 | 103.1 | 103.1 | 3.053 | 0.0 | 0.2 | 5 | OOO | C | yes | -259 | [39] |
| 49. | 1.983 | 1.981 | 1.958 | 1.977 | 102.0 | 101.4 | 101.7 | 3.063 | 5.3 | 0.9 | 4 | NN | C | | -710 | [40] |
| 50. | 2.012 | 1.854 | 2.012 | 1.854 | 96.1 | 107.7 | 101.9 | 2.993 | 0.0 | 7.9 | 4 | NS | C | | -809 | [41] |
| 51. | 1.912 | 1.895 | 1.929 | 1.927 | 98.8 | 99.5 | 99.2 | 2.917 | 0.4 | 5.6 | 4 | NN | H | | -130 | [42] |
| 52. | 1.941 | 1.948 | 1.917 | 1.947 | 97.2 | 96.0 | 96.6 | 2.894 | -4.6 | 4.3 | 5 | NNO | H | | 49 | [43] |
| 53. | 1.904 | 1.924 | 1.927 | 1.917 | 100.4 | 100.0 | 100.2 | 2.942 | 3.1 | 3.5 | 4/5 | OO/NNO | C | | -650 | [44] |
| 54. | 1.963 | 1.963 | 1.963 | 1.963 | 99.3 | 99.3 | 99.3 | 2.992 | 0.0 | 16.9 | 4 | NN | H | | -175 | [45] |
| 55. | 1.902 | 1.902 | 1.902 | 1.902 | 104.4 | 104.4 | 104.4 | 3.000 | 0.0 | 5.8 | 4 | NN | H | | -509 | [46] |
| 56. | 1.921 | 1.969 | 1.969 | 1.921 | 103.3 | 103.3 | 103.3 | 3.051 | 0.0 | 0.9 | 5 | NOO | C | | -690 | [47] |
| 57. | 1.969 | 1.982 | 1.982 | 1.969 | 97.5 | 97.5 | 97.5 | 2.970 | 0.0 | 16.9 | 5 | NNI | C | | -65 | [48] |
| 58. | 1.97 | 1.969 | 1.969 | 1.97 | 103.6 | 103.6 | 103.6 | 3.096 | 0.0 | 2.2 | 6 | NNOO | C | | -850 | [49] |
| 59. | 2.405 | 1.928 | 2.379 | 1.93 | 78.8 | 103.8 | 91.3 | 3.035 | -26.4 | 96 | 5 | NNO | H ₂ /H | | 19.3 | [50] |
| 60. | 1.922 | 1.923 | 1.923 | 1.922 | 99.7 | 99.7 | 99.7 | 2.939 | 0.0 | 0.1 | 5 | NOO | C | yes | -387 | [51] |
| 61. | 2.005 | 2.013 | 2 | 1.991 | 94.9 | 94.9 | 94.9 | 2.951 | 21.8 | 2 | 6 | NOOO | C/Mo | yes | 38 | [52] |
| 62. | 2.819 | 1.934 | 1.934 | 2.819 | 96.5 | 96.5 | 96.5 | 3.594 | 0.0 | 3.2 | 6 | NCIO | N | | 9.2 | [53] |
| 63. | 1.918 | 1.927 | 1.927 | 1.918 | 103.9 | 103.9 | 103.9 | 3.028 | 0.0 | 11.2 | 5 | NNO | C | yes | -390 | [54] |
| 64. | 1.955 | 1.948 | 1.947 | 1.962 | 96.6 | 96.4 | 96.5 | 2.914 | -12.5 | 1.8 | 4 | NN | H | yes | 12 | [55] |
| 65. | 1.916 | 1.93 | 1.923 | 1.934 | 97.7 | 96.9 | 97.3 | 2.891 | 0.1 | 1.4 | 4 | NN | H | | 158 | [56] |
| 66. | 1.97 | 1.946 | 1.956 | 1.96 | 103.8 | 104.5 | 104.2 | 3.089 | -2.5 | 5.4 | 5 | NNO | C | | -828 | [57] |
| 67. | 1.962 | 1.931 | 1.931 | 1.962 | 102.5 | 102.5 | 102.5 | 3.035 | 0.0 | 7.3 | 5 | NOO | C | | -82.5 | [58] |
| 68. | 1.926 | 1.968 | 1.968 | 1.926 | 101.1 | 101.1 | 101.0 | 3.007 | 0.0 | 27.5 | 4 | NO | C | | -166 | [59] |
| 69. | 1.943 | 1.918 | 1.918 | 1.943 | 98.3 | 98.3 | 98.3 | 2.919 | 0.0 | 46 | 4 | OO | C | yes | -131.6 | [60] |
| 70. | 2.273 | 1.992 | 1.972 | 2.394 | 97.5 | 93.2 | 95.3 | 3.197 | -22.9 | 62.8 | 5 | NNO | C | yes | 154 | [61] |
| 71. | 1.96 | 1.953 | 1.965 | 1.9 | 100.5 | 103.1 | 101.8 | 3.017 | -0.9 | 27.4 | 4 | NN | C | | -753 | [62] |
| 72. | 2.026 | 1.917 | 1.97 | 1.94 | 100.2 | 105.3 | 102.7 | 3.066 | 3.2 | 29.0 | 5 | NNN | C | | -610 | [62] |
| 73. | 1.944 | 1.942 | 1.942 | 1.944 | 95.6 | 95.6 | 95.6 | 2.880 | 0.0 | 0.5 | 5 | NNO | H | | 114 | [63,64] |
| 74. | 1.962 | 1.89 | 1.953 | 1.887 | 97.2 | 102.1 | 99.7 | 2.937 | 13.3 | 12.4 | 4 | NO | C | | -443 | [65] |
| 75. | 1.918 | 2.004 | 1.933 | 1.942 | 105.0 | 101.0 | 103.0 | 3.055 | -1.0 | 1.3 | 5 | NCICl | C/Cu | yes | -822 | [65] |
| 76. | 1.966 | 1.93 | 1.953 | 1.916 | 100.3 | 103.0 | 101.7 | 3.010 | -10.5 | 7.3 | 4 | NN | C | | -664 | [65] |
| 77. | 1.946 | 1.952 | 1.952 | 1.946 | 98.3 | 98.3 | 98.3 | 2.948 | -12.2 | 14.6 | 5 | NNO | C | | -128 | [66] |
| 78. | 1.913 | 1.986 | 1.919 | 1.97 | 103.0 | 98.6 | 100.8 | 2.999 | -3.4 | 26.5 | 5 | NBrBr | C/Cu | yes | -296 | [67] |
| 79. | 1.947 | 2.007 | 1.932 | 1.942 | 100.8 | 98.3 | 99.5 | 2.988 | 3.6 | 13 | 5 | NOO | C/Cu ₂ | yes | -174 | [67] |
| 80. | 1.891 | 1.922 | 1.922 | 1.891 | 103.9 | 103.9 | 103.9 | 3.003 | 0.0 | 9.5 | 4 | NN | C | | -560 | [68] |
| 81. | 2.257 | 1.975 | 1.975 | 2.257 | 102.2 | 102.2 | 102.2 | 3.299 | 0.0 | 65.8 | 5 | NOO | C | yes | 34.4 | [69] |
| 82. | 1.996 | 1.971 | 1.958 | 1.96 | 102.3 | 103.2 | 102.7 | 3.079 | 2.5 | 6.5 | 5 | NNO/NNCI | C | yes | -698 | [70] |
| 83. | 1.976 | 1.91 | 1.974 | 1.902 | 95.0 | 99.6 | 97.3 | 2.912 | -1.2 | 29.1 | 5 | NNN | C | | -77.05 | [71] |
| 84. | 1.968 | 1.927 | 2 | 1.927 | 95.0 | 98.8 | 96.9 | 2.926 | -2.1 | 29.0 | 5 | NNN | C | | -73.9 | [71] |
| 85. | 1.984 | 1.926 | 2.032 | 1.908 | 94.7 | 100.7 | 97.7 | 2.953 | -2.3 | 23.8 | 5 | NNN | C | | -117.4 | [71] |
| 86. | 1.902 | 1.908 | 1.908 | 1.902 | 103.2 | 103.2 | 103.2 | 2.986 | 0.0 | 5.0 | 4 | NN | C | | -600 | [72] |
| 87. | 1.962 | 1.962 | 1.962 | 1.962 | 105.3 | 105.3 | 105.3 | 3.120 | 0.0 | 13.8 | 6 | NNOO | C | yes | -490 | [73] |
| 88. | 1.953 | 2.445 | 2.65 | 1.952 | 95.7 | 102.6 | 99.2 | 3.445 | 11.8 | 70.5 | 5/6 | NOO/NOOO | C | | 0.63 | [74] |
| 89. | 1.933 | 1.952 | 1.965 | 1.897 | 101.1 | 102.9 | 102.0 | 3.011 | -0.5 | 5.7 | 4/5 | NN/NNO | C/H | | -529 | [75] |
| 90. | 1.933 | 1.924 | 1.924 | 1.933 | 103.6 | 103.6 | 103.6 | 3.031 | 0.0 | 0.8 | 5 | NNO | C | | -860 | [76] |
| 91. | 2.032 | 1.982 | 1.977 | 2.057 | 97.0 | 96.1 | 96.6 | 3.003 | -15.9 | 23.0 | 6 | NNNO | C/Cu | yes | -144 | [77] |
| 92. | 1.961 | 1.969 | 1.969 | 1.961 | 101.6 | 101.6 | 101.6 | 3.046 | 0.0 | 7.5 | 5 | NNN | C | | -241 | [78] |
| 93. | 2.44 | 1.921 | 1.921 | 2.44 | 94.3 | 94.3 | 94.3 | 3.218 | 0.0 | 67 | 5 | NNN | C | | 1.6 | [79] |
| 94. | 1.941 | 1.903 | 1.909 | 1.97 | 92.8 | 92.1 | 92.4 | 2.788 | 17.3 | 13.8 | 4 | NN | C | | -25.2 | [80] |
| 95. | 1.949 | 1.986 | 1.986 | 1.949 | 101.6 | 101.6 | 101.6 | 3.050 | 0.0 | 11.4 | 5 | NOO | C | | -182 | [81] |
| 96. | 1.942 | 1.985 | 1.985 | 1.942 | 102.5 | 102.5 | 102.5 | 3.062 | 0.0 | 11.7 | 5 | NOO | C | | -210 | [81] |
| 97. | 1.975 | 1.974 | 1.974 | 1.975 | 103.7 | 103.7 | 103.7 | 3.105 | 0.0 | 2.7 | 5 | NNI | C | | -771 | [82] |
| 98. | 1.975 | 1.918 | 1.966 | 1.915 | 94.8 | 98.4 | 96.6 | 2.902 | 14.4 | 5.3 | 4 | NN | H | | 16 | [83] |
| 99. | 1.9 | 1.919 | 1.919 | 1.9 | 100.5 | 100.5 | 100.5 | 2.935 | 0.0 | 6.4 | 4 | NN | H | | -201 | [84] |
| 100. | 1.968 | 1.964 | 1.964 | 1.968 | 93.5 | 93.5 | 93.5 | 2.865 | 0.0 | 4.0 | 4 | NO | SrH | | -300 | [85] |
| 101. | 1.97 | 1.905 | 1.878 | 1.96 | 99.2 | 98.6 | 98.9 | 2.930 | -0.9 | 11.7 | 4 | NO | SrH/CCu | yes | -101 | [86] |
| 102. | 2.013 | 1.969 | 1.951 | 2.375 | 99.7 | 87.9 | 93.8 | 3.029 | 26.7 | 29 | 5 | NNO | C | | -15 | [87] |
| 103. | 1.931 | 1.932 | 1.932 | 1.931 | 95.3 | 95.3 | 95.3 | 2.854 | 0.0 | 2.2 | 4 | NNO | H | yes | 24.5 | [88] |
| 104. | 1.901 | 1.913 | 1.913 | 1.901 | 102.9 | 102.9 | 102.9 | 2.983 | 0.0 | 1.1 | 4 | NN | C | | -600 | [89] |
| 105. | 1.961 | 1.97 | 1.97 | 1.961 | 103.8 | 103.8 | 103.8 | 3.093 | 0.0 | 5.3 | 5 | NNN | CH | | -598.8 | [90] |
| 106. | 1.906 | 1.904 | 1.904 | 1.906 | 103.7 | 103.7 | 103.7 | 2.996 | 0.0 | 8.2 | 4 | NN | H | | -410 | [91] |
| 107. | 1.897 | 1.931 | 1.931 | 1.897 | 101.6 | 101.6 | 101.6 | 2.966 | 0.0 | 4.0 | 4 | NN | H | | -360 | [92] |
| 108. | 1.969 | 1.943 | 1.943 | 1.969 | 101.8 | 101.8 | 101.8 | 3.035 | 0.0 | 5.5 | 4 | NN | C | | -857 | [49] |

(continued)

Table 1. (continued)

| Structure ^B | B ₁ | B ₂ | B ₃ | B ₄ | ϕ_1 | ϕ_2 | ϕ | r | T_1 | T_2 | nL | CuL | R _μ | CL | 2J | Reference |
|------------------------|----------------|----------------|----------------|----------------|----------|----------|--------|-------|-------|-------|----|------|----------------|-----|------|-----------|
| 109. | 1.918 | 1.918 | 1.918 | 1.918 | 104.0 | 104.0 | 104.0 | 3.031 | 0.0 | 6.4 | 4 | NO | C | | -800 | [1] |
| 110. | 1.938 | 2.440 | 2.440 | 1.938 | 95.9 | 95.9 | 95.9 | 3.269 | 0.0 | 1.8 | 6 | NNOO | Cu/H | | -313 | [93] |
| 111. | 1.899 | 1.931 | 2.455 | 2.450 | 75.7 | 103.6 | 89.6 | 3.009 | 19.8 | 61.2 | 5 | NOO | C/H | yes | -373 | [94] |
| 112. | 1.957 | 1.940 | 1.968 | 1.939 | 101.0 | 100.9 | 101.0 | 3.014 | 4.8 | 1.2 | 4 | NN | C/H | | -516 | [95] |
| 113. | 1.89 | 1.96 | 1.96 | 1.89 | 104.6 | | 104.6 | 3.047 | | | 4 | NBr | C | | -410 | [96] |
| 114. | 1.915 | 1.992 | 1.992 | 1.915 | 102.2 | | 102.2 | 3.041 | | | 4 | NCl | C | | -292 | [15] |
| 115. | 1.92 | 1.945 | 1.938 | 1.928 | 99.3 | 98.1 | 98.7 | 2.940 | | | | | | | -3.8 | [33] |
| 116. | | | | | 96.4 | | 96.4 | 2.870 | | | 4 | NN | H | | 145 | [97] |
| 117. | | | | | 106.3 | 100.6 | 103.5 | 3.018 | | | 4 | NN | C/H | | -852 | [98] |

^AIf the two copper (oxygen) atoms have different ligands, these are separated by a slash, else both the copper (oxygen) atoms have the same type of atoms connected. The schematic structure for the description of molecule is shown in the diagram; missing structural parameters in the table indicate that the data was taken from magnetism reports.

^BStructure numbers are as follows:

1. Bis(*N*-(3-hydroxypropyl)-3-nitrosalicylaldiminato-copper(II))
2. Bis(benzoylacetylacetonato)-bis(py)-di-copper(II) pyridine solvate
3. Dichloro-bis(μ_2 -(2-(2-dimethylamino)ethylthio)ethanol)-di-copper(II)
4. Dichloro-bis(μ_2 -(2-(2-diethylamino)ethylthio)ethanol)-di-copper(II)
5. Dichloro-bis(μ_2 -(2-(2-dipropylamino)ethylthio)ethanolato-*N, O, O', S*)-di-copper(II)
7. Dibromo-bis(μ_2 -(2-(2-dipropylamino)ethylthio)ethanol)-di-copper(II)
8. Bis(μ_2 -ethoxo)-bis(*O*-(1-oxy-2,2,6,6-tetramethylpiperidin-4-yl)pivaloylacetato-*O, O'*)-di-copper(II)
9. (μ_2 -Hydroxy)-(2,6-bis(bis(2-(1-pyrazolyl)ethyl)amino)methyl)-*p*-cresolato)-di-copper(II) bis(tetrafluoroborate)
10. Aqua-(μ_2 -hydroxo)-(μ_2 -1,5-bis(1-(pyridin-2-yl)-methylideneamino)-pentan-3-olato)-di-copper(II) diperchlorate monohydrate
11. Bis(bromo-(μ_2 -(2-(2-dimethylamino)-ethylthio)-ethanolato)-*N, S, O, O*)-copper(II)
12. Bis(bipyridyl)-di- μ -hydroxo-di-copper(II) nitrate
13. Bis(μ -*N-n*-butyl-(5-chloro- α -phenyl-2-hydroxy-benzylidene)-aminato)-bis(bromo-copper(II))
14. Bis(2,2-dimethyl-7-(phenylimino)-3,5,7-octanetrionato)-di-copper(II) benzene solvate
15. Bis(μ_2 -6-acetyl-7-oxo-4-aza-octen-1-olato-*N, O, O'*)-di-copper
16. Di- μ -(benzyl-oxo)-bis(2,2,6,6-tetramethylheptane-3,5-dionato-copper(II))
17. Bis(μ_2 -*N*-(propanolato)- α -aminoisobutyramide-*N, N', O*)-di-copper
18. *Trans*-bis(chloro-(*N*-ethylsalicylaldimino)-copper(II))
19. Bis(chloro-(*N*-isopropyl-salicylaldiminato)-copper(II))
20. ((μ_2 -hydroxo)-((μ_2 -2,6-bis(2-(2-pyridyl)ethyl)amine-methyl)-phenoxo-*N, N, N, O, O*)-di-copper(I) bis(hexafluorophosphate)
21. Bis(*N*-(3-hydroxypropyl)-5-chlorosalicylaldiminato-copper(II))
22. Di- μ -hydroxo-bis(2-(2-dimethylaminoethyl)pyridyl) di-copper(II) perchlorate form
23. Bis(hexafluoroacetylacetonato)-copper(II)-(*N, N'*-ethylene-bis(2-hydroxy-propiofenone-iminato)-copper(II)) inic form
24. μ -(*N, N'*-ethylene-bis(salicylideneiminato))-bis(hexafluoroacetylacetonato)-di-copper(II)
25. Di- μ -hydroxo-bis(bipyridyl)-copper(II) perchlorate
26. Aqua(μ_2 -2,6-bis(3-(dimethylamino)-propyliminomethyl)-4-methyl-phenolato-*N, N', N'', N''', O*)-(2-hydroxo)-perchlorato-copper perchlorate
27. Bis(μ_2 -acetato)-bis(7-amino-4-methyl-5-aza-hept-3-en-2-onato)-di-copper(II)
28. Bis(dimethylsulfoxide-*O*)-(2-(1,3,5,7-tetra-azabicyclo(3.3.1)nonan-3-yl)-ethanolato-*N_3, N_7, O*)-copper(II) diperchlorate
29. Bis(dimethylsulfoxide-*O*)-(2-(7-methoxymethyl-1,3,5,7-tetra-azabicyclo(3.3.1)nonan-3-yl)-ethanolato-*N_3, N_7, O*)-copper(II) diperchlorate
30. Bis(perchlorato-*O*)-(2-(1,3,5,7-tetra-azabicyclo(3.3.1)nonan-3-yl)-propanolato-*N_3, N_7, O*)-copper(II)
31. Bis(μ_2 -*N*-tosylglycinato-*O*)-bis(*N*-tosylglycinato-*O*)-bis(2,2'-bipyridyl)-di-copper(II) dihydrate
32. (μ_2 -hydroxo-*O, O*)-(2-(2,6-bis(bis(2-(methylthio)-ethyl)-aminomethyl)-4-methylphenol-*N, O, O, S, S'*)-di-copper(II) diperchlorate
33. Bis(μ_2 -acetato-*O, O*)-bis(μ_2 -acetato-*O, O'*)-bis(*N*-methyl-*N'*-(4-methoxysalicylidene)-1,3-propanediamine)-tri-copper(II)
34. (μ_3 -Hydroxo)-tris(μ -7-amino-4-methyl-5-aza-hept-3-en-2-onato-*N, N', O, O*)-tri-copper(II) diperchlorate
35. Bis(μ_2 -acetato-*O, O, O'*)-bis(*N*-methyl-*N'*-(5-nitrosalicylidene)-1,3-propanediamine-*N, N', O*)-di-copper(II)
36. Bis(μ_2 -acetato-*O, O, O'*)-bis(*N*-methyl-*N'*-(5-bromosalicylidene)-1,3-propanediamine-*N, N', O*)-di-copper(II)
37. Bis(μ_2 -acetato-*O, O*)-bis(*N*-methyl-*N'*-(5-methoxysalicylidene)-1,3-propanediamine-*N, N', O*)-di-copper dihydrate
38. (μ_2 -hydroxo)-(μ_2 -perchlorato-*O, O'*)-(2-(2,6-bis(*N*-(2-pyridylmethyl)-formidoyl)-4-methylphenolato-*O, O, N, N', N'', N'''*)-di-copper(II) perchlorate
39. Aqua-(μ_2 -hydroxo)-(μ_2 -2,6-bis(*N*-(2-pyridylmethyl)-formidoyl)-4-methylphenolato-*O, O, N, N', N'', N'''*)-di-copper(II) dinitrate
40. Bis(*N*-(2-ethylthioethyl)-3-aminopropanolato-*S, N, O*)-dichloro-di-copper(II) dihydrate
41. (μ_2 -cyanato-*O*)-(2-(2,6-bis(*N*-(2-dimethylaminoethyl)-methylimino-*N, N'*)-4-methylphenolato-*O*))-di-copper(II) diperchlorate
42. (μ_2 -2,6-bis(5'-amino-1'-methyl-2'-azapent-1'-enyl)-4-methylphenolato-*O, N, N', N'', N'''*)-(2-hydroxo)-di-copper(II) diperchlorate monohydrate
43. Bis(μ -9,9,9-trifluoro-8-(trifluoromethyl)-6-methyl-5-aza-non-5-ene-1,8-diolato- μ -*O, N, O'*)-di-copper(II)
44. Bis(μ -8,8,8-trifluoro-7-(trifluoromethyl)-5-methyl-4-aza-oct-4-ene-1,7-diolato- μ -*O, N, O'*)-di-copper(II)
45. (μ_2 -2-(2-(2-(*o*-hydroxy- α -methylbenzylidene)amino)ethyl)amino)-ethanol-*N, N', O, O'*)-(2-(2-(2-(*o*-hydroxy- α -methylbenzylidene) amino)ethyl)amino)-ethanolato-*N, N', O, O'*)-di-copper(II) perchlorate
46. Bis(μ_2 -*N*-phenylsalicylaldiminato-*N, O*)-chloro-copper(II))
47. (μ_2 -cyanato)-(μ_2 -2,6-bis(*N*-(2-pyridylmethyl)formimidoyl)-4-methylphenolato-*N, N', N'', N'''*)-*O*)-di-copper(II) diperchlorate
48. Tetrakis(μ_2 -acetato-*O, O'*)-bis(μ_3 -3-(4-(2-pyridyl)-2-azabut-1-enyl)catecholato-*O, O, O', O', N, N'*)-tetra-copper(II) monohydrate
49. (μ_2 -11,23-trifluoromethyl-3,7,15,19-tetra-azatricyclo(19.3.1.19.13) hexacos-1(25),2,7,9,11,13(26),14,19,21,23-decaene-25,26-diolato)-di-copper(II) diperchlorate
50. (μ_2 -2,6-bis(4-(2-benzimidazolyl)-2-thiabutyl)-4-methylphenolato-*N, N', S, S', O, O*)-(2-hydroxo)-diperchlorato-copper(II) methanol solvate

(continued)

Table 1. (continued)

51. Di- μ -hydroxo-bis(2-(2-ethylaminoethyl)pyridyl) di-copper(II) perchlorate
52. (2,2'-Bipyridyl-aqua-copper(II))-bis(μ_2 -hydroxo)-(2,2'-bipyridyl-sulfato-copper(II)) tetrahydrate
53. (*N,N'*-bis(2-Hydroxylato-3-carboxylato-benzylidene)-1,2-diaminoethane)-methanol-di-copper(II)
54. Bis(μ_2 -hydroxo)-bis(bis(2-methylimidazole)-copper(II)) diperchlorate dihydrate
55. Bis(μ -hydroxo)-bis(*N,N,N',N'*-tetramethylethylenediamine)-di-copper(II) dibromide
56. Bis(heptanetronato)-bis(pyridyl) copper(II)
57. *Catena*- μ -iodo-bis(μ -(2-(3-aminopropyl)-amino)-ethanolato-*N,N',O*)-copper(II) iodide dihydrate
58. Bis(aqua-*N,N'*-bis(μ_2 -4-methyl-2,6-diformylphenolato-*O*)-(1,3-diaminopropano-*N,N'*)-copper(II)) bis(aqua-*N,N'*-bis(μ_2 -4-methyl-2,6-diformylphenolato-*O*)-(1,3-diaminopropano-*N,N'*)-perchlorato-copper(II)) diperchlorate
59. (μ_2 -acetato-*O,O'*)-(μ_2 -aqua)-(μ_2 -hydroxo)-bis((2,2'-bipyridyl)-copper(II)) diperchlorate
60. *Catena*(bis(μ_2 -3-amino-1-propanol-*N,O*)-(nitrato-*O,O'*)-copper(II)))
61. (*Catena*-bis(μ_4 -1,3-dihydroxy-2-methyl-2-(salicylideneamino)propane)-bis(μ_3 -methoxo)-(μ_2 -oxo)-tri-oxo-di-copper-di-molybdenum acetonitrile solvate)
62. Bis(μ_2 -chloro)-bis(μ_2 -2,2'-(1,2-ethanediyl)-bis(nitrilomethylidene))-bis(pyridine-*N*-oxide-*N,N',O,O'*)-di-copper(II)-bis(trichloro-zinc)
63. Bis(μ_2 -acetato-*O,O'*)-bis(μ_2 -methoxo)-bis(μ_2 -*N,N'*-propane-bis(salicyclideneiminato-*N,N',O,O,O',O')*)-tetra-copper
64. Tetrakis(μ_3 -hydroxo)-(2,2'-bipyridyl-*N,N'*)-copper(II) hexafluorophosphate
65. Bis(μ_2 -hydroxo)-bis((2,2'-bipyridyl)-copper(II)) bis(trifluoromethanesulfonate)
66. (μ_2 -5,17-Dihydroxy-11,23-dimethyl-3,7,15,19-tetra-aza-tricyclo(18.3.1.19,13) hexacos-2,7,9,11,13(26),14,19,21,23,1(25)-decaene-25,26-diolato)-methanol-perchlorato-di-copper(I,II) perchlorate
68. Bis(nitrato-*N*-ethyl-2-hydroxybenzylidenediminato)-copper(II)); Di- μ -(*N*-ethylsalicylaldiminato)bis (nitrato-copper(II))
69. Bis(perfluoro-*tert*-butoxy)-hexakis(μ_2 -*tert*-butoxo)-tetra-copper
70. Aqua-(μ_3 -acetato-*O,O,O'*)-bis(μ_2 -acetato-*O,O'*)-(acetato-*O*)-tris(2,2'-bipyridyl)-tri-copper(II) bis(hexafluorophosphate)
71. Bis(μ_2 -2,6-(pyridazine-1,4-bis(thioethyliminomethyl)-4-methylphenoxo-*N,N',O,O:N,N',N'',O,O*))-di-copper(I,II) tetrakis(tetrafluoroborate) dihydrate
72. Bis(μ_2 -2,6-(pyridazine-1,4-bis(thioethyliminomethyl)-4-*t*-butyl-phenoxo-*N,N',O,O:N,N',N'',O,O*))-di-copper(I,II) bis(tetrafluoroborate) methanol solvate
73. Bis((μ_2 -hydroxo)-aqua-(2,2'-bipyrimidinyl-*N,N'*)-copper(II)) dinitrate tetrahydrate
74. (Bis(nitrato)-(μ_2 -methoxo)-(μ_2 -9-methyl-2,16,5,13,18,19-dithiatetra-azatricyclo(15.2.2.17,11) docosa-1(19),5,7,9,11(22),12,17,20-octaen-22-olato-*N,N',O,O*))-di-copper
75. Dichloro-bis((μ_3 -methoxo)-(μ_2 -chloro)-(μ_2 -9-methyl-2,16,5,13,18,19-dithiatetra-azatricyclo(15.2.2.17,11)docosa-1(19),5,7,9,11(22),12,17,20-octaen-22-olato-*N,N',O,O*))-di-copper
76. Tetrakis(thiocyanato)-bis((μ_3 -methoxo)-(μ_2 -9-methyl-2,16,5,13,18,19-dithiatetra-azatricyclo(15.2.2.17,11)docosa-1(19),5,7,9,11(22),12,17,20-octaen-22-olato-*N,N',O,O*))-di-copper
77. Bis(*N*-picolinoyl-3-amino-1-propanolato)-aqua-copper(II) dihydrate
78. (μ_4 -Oxo)-tetrakis(μ_2 -bromo)-bis(μ_2 -2,6-bis(morpholinomethyl)-4-methylphenolato)-tetra-copper(II) methanol solvate
79. (μ_4 -Oxo)-tetrakis(μ_2 -benzoato-*O,O'*)-bis(μ_2 -2,6-bis(morpholinomethyl)-4-methylphenolato)-tetra-copper(II) monohydrate
80. (Pyrrole-2-(*N*-3-propanolato)-carboxaldimino) copper(II)
81. Bis(μ_2 -di-2-pyridylmethanediol-*N,N',O,O*)-bis(μ_3 -acetato-*O,O,O'*)-bis(μ_2 -acetato-*O,O'*)-bis(acetato-*O*)-tetra-copper dichloromethane solvate dihydrate
82. *Catena*-(tetrakis(μ_2 -chloro)-bis(μ_3 -*N,N'*-bis(2-hydroxyformamide-6-formyl-4-methylphenolato)-1,3-diaminopropane)-hexa-copper(I,II))
83. (μ_2 -1,5-Bis(bis((1-methyl-4-imidazolyl)methyl)amino)-3-pentanolato)-(μ_2 -ethoxo)-di-copper(II) diperchlorate acetonitrile solvate
84. (μ_2 -1,5-bis(bis((1-methyl-4-imidazolyl)methyl)amino)-3-pentanolato)-(μ_2 -isopropoxo)-di-copper(II) diperchlorate dichloromethane solvate
85. (μ_2 -1,5-bis(bis((1-isopropyl-4-imidazolyl)methyl)amino)-3-pentanolato)- (μ_2 -methoxo)-di-copper(II) diperchlorate dichloromethane methanol solvate
86. Bis(μ_2 -methoxo)-bis(bis(1-methyl-2-benzimidazolyl)propane)-di-copper(II) diperchlorate
87. Bis(μ_2 -methoxo)-tetrakis((methoxy)-bis(2-pyridyl)methanol)-tetra-copper(II) diperchlorate
88. Bis(μ_2 -acetoxo)-bis(*N*-(1,1-dimethyl-2-hydroxyethyl)-salicylaldiminato)-copper(II) ethanol solvate monohydrate
89. Aqua-(μ_2 -hydroxo)-(μ_2 -2,6-bis(*N*-(2-(imidazol-4-yl)ethyl)iminomethyl)-*p*-cresolato-*N,N',N'',N''',O,O*))-di-copper(II) perchlorate
90. (μ_2 -3,13-Dimethyl-3,13-dinitro-1,5,11,15-tetra-azaicosane-8,18-diolato)-bis(nitrito-*O*)-copper(II) monohydrate
91. Bis(μ_2 -acetato-*O,O'*)-octakis(μ_2 -dihydroxy-di-2-pyridylmethane)-diacetato-octa-copper(II) tetra-perchlorate nonahydrate
92. Bis(μ_2 -*N*-(2-hydroxybenzyl)-1,4,7-triazacyclononane-*N*-acetato-*O,O'*)-di-copper(II) diperchlorate
93. Bis((μ_2 -*N*-(salicylidene)-*N'*-(1-triphenylborylimidazol-2-ylmethylene)-1,3-propanediamino)-copper(II))
94. (μ_2 -7,18-Bis(acetonyl)-10,21-dimethyl-23,24-dihydroxy-4,5,15,16-tetracyano-3,6,14,17-tetra-azatricyclo(17.3.1.18,12)tetracos-1(23),2,4,8,10,12(24),13,15,19,21-Decene)-di-copper(II) acetone solvate
95. Bis(acetato(μ_2 -2-(1,5-diazabicyclo(3.2.1)oct-8-yl)phenoxo-*O,O,N*)-ethanol-copper(II))
96. Bis(acetato-(μ_2 -2-(1,5-diazabicyclo(3.2.1)oct-8-yl)phenoxo-*O,O,N*)-methanol-copper(II))
97. (Bis(1,3-diaminopropane-*N,N'*)-bis(4-methyl-2,6-diformylphenolato)-*O,O,N,N'*)-di-iodo-di-copper(II) monohydrate
98. Bis(μ_2 -hydroxo)-(1,10-bis(2,2'-bipyridyl-5-ylcarbonyl)-1,10-diaza-4,7,13,16-tetraoxacyclo-octadecane-*N,N',N'',N'''*)-di-copper(II) bis(tetrafluoroborate) dihydrate
99. Di- μ -hydroxo-bis(2-(2-dimethylaminoethyl)pyridyl) di-copper(II) perchlorate
100. Bis(μ_3 -hydroxy)-hexakis(μ_2 -1,3-bis(dimethylamino)-2-propanolato-*N,N',O*)-tetrakis(trifluoroacetato-*O*)-tetra-copper(II)-di-strontium tetrahydrofuran solvate
101. (μ_4 -Oxo)-bis(μ_2 -2,6-bis((dimethylamino)methyl)-4-methylphenolato-*N,N',O*)-tetrakis(trifluoroacetato-*O*)-tetra-copper(II))
102. (μ_2 -Acetato-*O,O'*)-(acetato-*O*)-(2-(2-pyridylethylimino)-6-((4-methylpiperazin-1-yl)methyl)phenolato)-di-copper(II) perchlorate
103. Bis(μ_3 -carbonato-*O,O,O'*)-bis(μ_2 -hydroxo)-decakis(2,2'-bipyridyl-*N,N'*)-hexa-copper(II) hexaperchlorate tetrahydrate
104. Bis((μ_2 -methoxo)-(1,3-bis(2-benzimidazolyl)propane)-copper(II)) diperchlorate methanol solvate
105. (Dithiocyanato-*N*)-(3,15-di-*t*-butyl-25,26-dihydroxy-9,21-dioxo-7,11,19,23-tetra-azapentacos-1,3,5(25),6,11,13,15,17(26),18,23-decaene)-di-copper(II)

(continued)

Table 1. (continued)

106. Di- μ -hydroxo-bis(*N,N,N',N'*-tetramethylethylenediamine-copper(II)) perchlorate
 107. Di- μ -hydroxo-bis(*N,N,N',N'*-tetramethylethylenediamine-copper(II)) perchlorate
 108. Bis(*N,N'*-bis(μ_2 -4-methyl-2,6-diformylphenolato-*O,O'*)-(1,4-diaminobutano-*N,N'*)-copper(II))
 109. Bis(*N*-(3-hydroxypropyl)-5,6-benzosalicylaldiminato-copper(II))
 110. Bis($(\mu_3$ -hydroxo)-(μ_2 -1,4-bis(2-pyridylthio)phthalazine)-aqua-tris(nitrato-*O*)-di-copper)
 111. (μ_2 -Aqua)-(μ_2 -acetato-*O,O'*)-bis($(\mu_2$ -acetato-*O,O'*)-(μ_2 -hydroxo)-(μ_2 -1,3-bis(dimethylamino)-2-propanolato-*N,N',O,O'*)-di-copper(II)) hexafluorophosphate dichloromethane solvate
 112. (μ_2 -Hydroxo)-(μ_2 -2,6-(*N,N'*-bis(2-(4-imidazolyl)ethyl)-amino-methyl)-p-cresolato-*O,N,N'*)-di-copper diperchlorate sesquihydrate
 113. Dibromo-bis(*N*-ethylsalicylaldimino)-di-copper(II)
 114. *Trans*-bis(chloro(*N*-methylsalicylaldimino)-copper(II))
 115. (μ_2 -2,6-Bis(*N*-(2-dimethylaminoethyl)-methylimino-*N,N'*)-4-methylphenolato-*O,O'*)-(μ_2 -hydroxo)-di-copper(II) diperchlorate hydrate
 116. *Catena*-bis(μ_2 -hydroxo)-(μ_2 -*squarato-O,O'*)-bis(2,2'-bipyridyl)-di-copper(II) tetrahydrate
 117. (μ_2 -2,6-Bis(diethylaminoethyliminomethyl)-4-methylphenolato-*N,N',N'',N''',O*)-(μ_2 -hydroxo)-di-copper(II) diperchlorate

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