

Crystal structure of *catena*-poly[(μ -2-aminopyrimidine-*N,N'*)bis(μ -chloro)-bis(triphenylphosphine)dicopper(I)], $\text{Cu}_2\text{Cl}_2[\text{P}(\text{C}_6\text{H}_5)_3]_2(\text{C}_4\text{H}_5\text{N}_3)$

Q.-H. Jin*, J.-C. Dong, H.-W. Gao, X.-L. Xin, L. Yang and P.-Z. Li

Capital Normal University, Department of Chemistry, Beijing 100037, P. R. China

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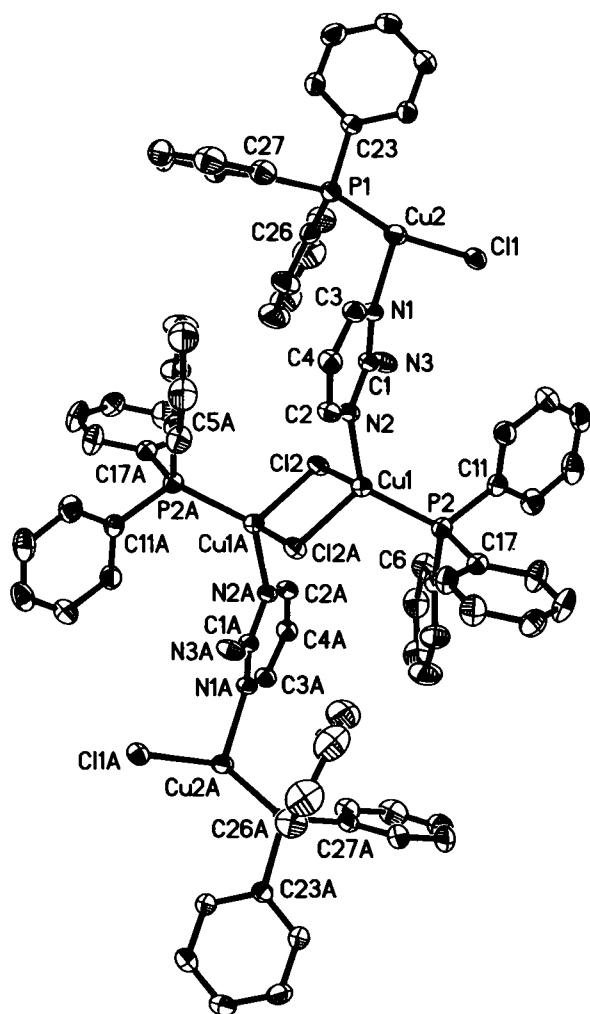


Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U _{iso}
H(3A)	2i	0.1150	0.4390	0.2953	0.063
H(3B)	2i	0.1930	0.4682	0.1886	0.063
H(3)	2i	0.3963	0.5089	0.4363	0.053
H(4)	2i	0.6055	0.5610	0.3123	0.058
H(2)	2i	0.6081	0.5762	0.1552	0.052
H(6)	2i	0.1285	0.5766	-0.0938	0.069
H(10)	2i	0.3809	0.8068	-0.2448	0.081
H(8)	2i	0.2529	0.6728	-0.3881	0.099
H(7)	2i	0.1269	0.5657	-0.2413	0.085
H(9)	2i	0.3864	0.7890	-0.3898	0.105
H(16)	2i	0.1052	0.6699	0.1604	0.063
H(15)	2i	-0.1326	0.6933	0.2481	0.080
H(14)	2i	-0.3202	0.7444	0.1718	0.081
H(13)	2i	-0.2734	0.7718	0.0058	0.085
H(12)	2i	-0.0341	0.7522	-0.0848	0.072
H(22)	2i	0.5211	0.7768	-0.0601	0.064
H(20)	2i	0.4362	1.0729	-0.1315	0.072
H(19)	2i	0.1960	1.0587	-0.1195	0.088

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(21)	2i	0.5985	0.9327	-0.1006	0.079
H(18)	2i	0.1182	0.9036	-0.0799	0.079
H(24)	2i	-0.1442	0.3232	0.6312	0.059
H(28)	2i	0.3589	0.3137	0.5866	0.069
H(31)	2i	0.3101	0.0566	0.5652	0.068
H(25)	2i	0.0895	0.0578	0.7094	0.066
H(29)	2i	0.5813	0.2447	0.6273	0.092
H(38)	2i	0.5305	-0.0124	0.6086	0.090
H(34)	2i	-0.3002	0.1054	0.8857	0.063
H(35)	2i	-0.3263	0.2652	0.7742	0.066
H(36)	2i	-0.0931	0.0011	0.8516	0.074
H(33)	2i	-0.0668	0.1335	0.5267	0.085
H(32)	2i	0.3127	0.2476	0.3588	0.085
H(37)	2i	0.6636	0.0822	0.6404	0.099
H(39)	2i	0.1039	0.1083	0.2627	0.117
H(40)	2i	0.2965	0.1960	0.2372	0.116
H(30)	2i	-0.0808	0.0809	0.4050	0.114

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu(1)	2i	0.40083(3)	0.57242(2)	0.04174(2)	0.0433(2)	0.0421(2)	0.0356(2)	-0.0007(2)	-0.0089(1)	-0.0124(2)
Cu(2)	2i	0.11962(4)	0.41768(2)	0.47902(2)	0.0504(2)	0.0403(2)	0.0377(2)	-0.0079(2)	-0.0028(2)	-0.0143(2)
Cl(2)	2i	0.34204(7)	0.41696(5)	0.04140(5)	0.0437(4)	0.0444(4)	0.0436(4)	-0.0091(3)	-0.0002(3)	-0.0211(3)
P(1)	2i	0.13508(7)	0.25231(5)	0.54177(5)	0.0407(4)	0.0386(4)	0.0386(4)	-0.0034(3)	-0.0063(3)	-0.0149(3)
P(2)	2i	0.25767(7)	0.69764(5)	-0.03521(5)	0.0409(4)	0.0393(4)	0.0385(4)	-0.0027(3)	-0.0139(3)	-0.0146(3)
Cl(1)	2i	-0.10966(7)	0.48587(5)	0.42441(5)	0.0453(4)	0.0587(4)	0.0404(4)	-0.0027(3)	-0.0102(3)	-0.0268(3)
N(1)	2i	0.2883(2)	0.4842(2)	0.3580(1)	0.040(1)	0.044(1)	0.029(1)	-0.006(1)	-0.0055(9)	-0.014(1)
N(2)	2i	0.4127(2)	0.5310(2)	0.1864(1)	0.038(1)	0.039(1)	0.030(1)	-0.005(1)	-0.0027(9)	-0.0134(9)
N(3)	2i	0.1893(2)	0.4633(2)	0.2475(2)	0.048(1)	0.082(2)	0.033(1)	-0.027(1)	-0.002(1)	-0.021(1)
C(1)	2i	0.2981(3)	0.4931(2)	0.2647(2)	0.036(2)	0.039(2)	0.032(1)	-0.003(1)	-0.005(1)	-0.014(1)
C(3)	2i	0.4016(3)	0.5121(2)	0.3731(2)	0.048(2)	0.052(2)	0.035(1)	-0.004(1)	-0.010(1)	-0.019(1)
C(4)	2i	0.5256(3)	0.5451(2)	0.2996(2)	0.040(2)	0.066(2)	0.043(2)	-0.014(1)	-0.008(1)	-0.023(1)
C(2)	2i	0.5257(3)	0.5536(2)	0.2065(2)	0.040(2)	0.049(2)	0.038(2)	-0.008(1)	-0.003(1)	-0.015(1)
C(5)	2i	0.2530(3)	0.6948(2)	-0.1535(2)	0.046(2)	0.053(2)	0.045(2)	0.005(1)	-0.019(1)	-0.022(1)
C(6)	2i	0.1785(3)	0.6211(2)	-0.1533(2)	0.067(2)	0.057(2)	0.062(2)	-0.000(2)	-0.028(2)	-0.028(2)
C(10)	2i	0.3299(4)	0.7575(3)	-0.2431(2)	0.078(2)	0.082(2)	0.048(2)	-0.017(2)	-0.017(2)	-0.022(2)
C(8)	2i	0.2542(4)	0.6773(3)	-0.3289(3)	0.096(3)	0.109(3)	0.066(3)	0.019(2)	-0.041(2)	-0.052(2)
C(7)	2i	0.1786(4)	0.6140(3)	-0.2417(3)	0.077(2)	0.083(3)	0.082(3)	0.007(2)	-0.038(2)	-0.051(2)
C(9)	2i	0.3319(4)	0.7476(3)	-0.3301(2)	0.102(3)	0.122(3)	0.042(2)	-0.020(3)	-0.015(2)	-0.028(2)
C(11)	2i	0.0629(3)	0.7099(2)	0.0281(2)	0.041(2)	0.037(2)	0.048(2)	-0.002(1)	-0.014(1)	-0.016(1)
C(16)	2i	0.0296(3)	0.6917(2)	0.1280(2)	0.048(2)	0.056(2)	0.055(2)	0.003(1)	-0.016(1)	-0.023(2)
C(15)	2i	-0.1132(4)	0.7051(2)	0.1811(2)	0.054(2)	0.071(2)	0.064(2)	-0.001(2)	-0.001(2)	-0.026(2)
C(14)	2i	-0.2242(4)	0.7351(2)	0.1359(3)	0.050(2)	0.045(2)	0.097(3)	-0.006(2)	0.005(2)	-0.031(2)
C(13)	2i	-0.1960(3)	0.7521(2)	0.0366(3)	0.043(2)	0.070(2)	0.107(3)	0.003(2)	-0.029(2)	-0.036(2)
C(12)	2i	-0.0528(3)	0.7400(2)	-0.0177(2)	0.050(2)	0.069(2)	0.066(2)	0.001(2)	-0.025(2)	-0.025(2)
C(17)	2i	0.3126(3)	0.8232(2)	-0.0670(2)	0.044(2)	0.041(2)	0.039(2)	-0.004(1)	-0.014(1)	-0.015(1)
C(22)	2i	0.4546(3)	0.8335(2)	-0.0726(2)	0.047(2)	0.044(2)	0.071(2)	0.000(1)	-0.018(2)	-0.023(2)
C(20)	2i	0.4047(4)	1.0101(2)	-0.1147(2)	0.071(2)	0.041(2)	0.069(2)	-0.013(2)	-0.023(2)	-0.013(2)
C(19)	2i	0.2622(4)	1.0018(2)	-0.1081(3)	0.080(3)	0.039(2)	0.104(3)	0.009(2)	-0.048(2)	-0.019(2)
C(21)	2i	0.5013(3)	0.9270(2)	-0.0967(2)	0.053(2)	0.054(2)	0.092(3)	-0.011(2)	-0.018(2)	-0.025(2)
C(18)	2i	0.2159(3)	0.9088(2)	-0.0843(2)	0.054(2)	0.044(2)	0.104(3)	-0.001(2)	-0.039(2)	-0.018(2)
C(23)	2i	-0.0067(3)	0.1973(2)	0.6546(2)	0.038(2)	0.044(2)	0.038(1)	-0.004(1)	-0.007(1)	-0.018(1)
C(27)	2i	0.3089(3)	0.1922(2)	0.5733(2)	0.041(2)	0.052(2)	0.035(1)	-0.002(1)	-0.004(1)	-0.015(1)
C(26)	2i	0.1233(3)	0.1972(2)	0.4555(2)	0.056(2)	0.038(2)	0.043(2)	0.003(1)	-0.017(1)	-0.016(1)
C(24)	2i	-0.1327(3)	0.2580(2)	0.6755(2)	0.048(2)	0.041(2)	0.050(2)	0.000(1)	-0.007(1)	-0.013(1)
C(28)	2i	0.3924(3)	0.2479(2)	0.5911(2)	0.053(2)	0.071(2)	0.053(2)	-0.008(2)	-0.015(2)	-0.024(2)
C(31)	2i	0.3633(3)	0.0946(2)	0.5788(2)	0.052(2)	0.054(2)	0.059(2)	0.004(2)	-0.009(2)	-0.023(2)
C(25)	2i	0.0061(3)	0.1003(2)	0.7220(2)	0.052(2)	0.045(2)	0.055(2)	0.003(1)	-0.007(2)	-0.012(1)
C(29)	2i	0.5258(4)	0.2065(3)	0.6157(2)	0.062(2)	0.114(3)	0.063(2)	-0.013(2)	-0.024(2)	-0.031(2)
C(38)	2i	0.4957(4)	0.0532(3)	0.6042(2)	0.059(2)	0.077(2)	0.067(2)	0.024(2)	-0.013(2)	-0.018(2)
C(34)	2i	-0.2272(3)	0.1282(2)	0.8275(2)	0.048(2)	0.066(2)	0.041(2)	-0.017(2)	-0.005(1)	-0.016(2)
C(35)	2i	-0.2420(3)	0.2233(2)	0.7615(2)	0.043(2)	0.064(2)	0.054(2)	-0.001(2)	-0.003(1)	-0.024(2)
C(36)	2i	-0.1032(3)	0.0664(2)	0.8073(2)	0.062(2)	0.054(2)	0.051(2)	-0.011(2)	-0.012(2)	0.001(2)
C(33)	2i	0.0074(4)	0.1465(3)	0.4684(2)	0.081(2)	0.083(2)	0.066(2)	-0.016(2)	-0.025(2)	-0.035(2)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(32)	2i	0.2323(4)	0.2143(2)	0.3686(2)	0.087(2)	0.074(2)	0.054(2)	-0.015(2)	-0.002(2)	-0.034(2)
C(37)	2i	0.5753(4)	0.1100(3)	0.6228(2)	0.047(2)	0.120(4)	0.060(2)	0.012(2)	-0.018(2)	-0.018(2)
C(39)	2i	0.1083(6)	0.1315(3)	0.3107(3)	0.166(5)	0.074(3)	0.080(3)	0.004(3)	-0.059(3)	-0.043(2)
C(40)	2i	0.2235(5)	0.1825(3)	0.2961(3)	0.143(4)	0.088(3)	0.058(2)	0.001(3)	-0.010(2)	-0.043(2)
C(30)	2i	-0.0007(5)	0.1143(3)	0.3957(3)	0.126(4)	0.095(3)	0.097(3)	-0.024(3)	-0.053(3)	-0.043(3)

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