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Structure Determination of the 2:1 Derivatives of Copper(I) Bromide and Iodide with Bis(diphenylphosphino)methane. A Simple Structural Scheme for the Formation of $(CuX)_nL_m$ Species

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The structures of the complexes $(CuX)_2DPM$ (X = Br, I; DPM = bis(diphenylphosphino)methane) were determined from three dimensional X-ray data collected by counter methods. The iodine derivative crystallizes in the space group Pbca with eight units in a cell defined by a = 17.128(9), b = 18.306(9), c = 16.508 (8) Å. The structure was refined by the least-squares method to a final R factor of 0.054 for 1336 non-zero independent reflections. The bromine derivative crystallizes in the space group $P2_1/c$ with eight units in a cell defined by a = 23.707(10), b = 17.805(9), c = 16.991(8) Å, β = 136.10(5)°. The final least-squares refinement, based on 2489 non-zero independent reflections, gave an R factor of 0.074.

Both the compounds have similar structures with a centrosymmetric $(CuX)_4$ core, in which two copper atoms have a tetrahedral geometry, while the other two are trigonal.

The above structures are compared with those already reported for other compounds $(CuX)_nL_m$ and a simple scheme is proposed to rationalize the different geometries of the $(CuX)_n$ core on the basis of steric and electronic effects.

Introduction

Many complexes between copper halides and neutral ligands, of general formula $(CuX)_nL_m$, are known. Often, as in the case of the series $(CuX)_nDPM_m$[1] (DPM = bis(diphenylphosphino)methane), they exist in different stoichiometric ratios, for the same X and L species, and show rather intriguing structures.

We report here the structures of the two compounds $(CuBr)_2DPM$ and $(CuI)_2DPM$. The preliminary results of the latter compound[2] and the data of the chlorine analogue[3] have already been published.

Our interest, considered the increasing importance of copper(I) chemistry in both the theoretical and preparative fields, is in studying the structural varieties of this element. On the basis of the present results and of the other known structures (see Table VI) we sug-

TABLE I. Crystal Data.

Compound	$(CuI)_2DPM$	$(CuBr)_2DPM$
Mol wt, amu	765.3	671.3
Cell dimensions, Å	a = 17.128 ± 0.009 b = 18.306 ± 0.009 c = 16.508 ± 0.008	a = 23.707 ± 0.010 b = 17.805 ± 0.009 c = 16.991 ± 0.008 β = 136.10 ± 0.05°
Density, g cm^{-3}		
obsd	1.94 ± 0.03[a]	1.82 ± 0.02[b]
calcd	1.96	1.79
Z	8	8
Space group	*Pbca*	$P2_1/c$
μ, cm^{-1}	43.0	53.9
Crystal dimensions, mm	0.15 × 0.15 × 0.20	0.40 × 0.40 × 0.60
Independent reflections	1336	2489
Final R	0.054	0.079

[a] Determined by flotation in dibromethane. [b] Determined by flotation in water solution of NaI.

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gest a simple scheme for the rationalization of the $(CuX)_nL_m$ structures known up to date.

Experimental

Collection and Reduction of Data

Specific details concerning crystal characteristics and X-ray diffraction methodology are summarized in Table I. The cell constants were determined by a least-squares fit of the diffractometer 2Θ, Φ and χ setting angles for 15 accurately centered reflections.

Intensity data for both structures were collected on a Siemens diffractometer with MoKα filtered radiation using Θ–2Θ scan technique. At regular intervals two reference reflections were measured in order to monitor the data collection. No changes in crystal or instrument performance were detected during data recording. Only the reflections with $I > 3\sigma(I)$ were used and corrected for background, Lorentz and polarization effects. The absorption correction was applied only for the bromine derivative. Atomic scattering factors were those given by Moore.[4]

TABLE II. Fractional Coordinates (x 10^4) and Temperature Factors of $(CuI)_2$DPM, with their Estimated Standard Deviations in Parentheses.

	X	Y	Z	B
I(1)	–695(2)	1463(1)	1363(1)	a
I(2)	1144(1)	186(1)	320(1)	a
Cu(1)	–101(2)	210(2)	1339(2)	a
Cu(2)	152(2)	–992(2)	35(2)	a
P(1)	94(4)	–590(4)	2326(4)	a
P(2)	160(4)	–1800(4)	1046(4)	a
CP	602(15)	–1392(14)	1958(15)	4.1(6)
C(1)	–752(16)	–900(14)	2924(15)	3.8(6)
C(2)	–1348(23)	–366(21)	2943(24)	8.4(11)
C(3)	–2053(21)	–667(21)	3500(22)	7.3(9)
C(4)	–2024(19)	–1212(20)	3847(21)	6.7(8)
C(5)	–1383(20)	–1737(10)	3842(21)	7.2(9)
C(6)	–707(19)	–1566(16)	3382(17)	5.5(7)
C(7)	730(16)	–186(15)	3081(16)	4.1(6)
C(8)	1524(19)	–351(17)	3051(20)	5.8(7)
C(9)	2072(18)	–51(17)	3609(19)	5.9(7)
C(10)	1760(18)	387(16)	4230(19)	5.7(7)
C(11)	960(20)	530(18)	4288(21)	6.7(8)
C(12)	431(15)	183(15)	3678(16)	4.3(6)
C(13)	–765(15)	–2234(13)	1378(16)	3.6(5)
C(14)	–739(18)	–2803(16)	1907(18)	5.5(7)
C(15)	–1419(18)	–3077(16)	2190(18)	5.4(7)
C(16)	–2125(20)	–2879(19)	1888(21)	6.6(8)
C(17)	–2134(18)	–2289(18)	1370(21)	6.6(7)
C(18)	–1436(20)	–1980(19)	1066(21)	6.9(8)
C(19)	778(14)	–2579(13)	842(14)	3.1(5)
C(20)	1482(19)	–2745(18)	1314(20)	6.0(8)
C(21)	1936(19)	–3303(18)	1078(20)	6.5(8)
C(22)	1729(17)	–3823(15)	443(17)	4.6(6)
C(23)	1034(22)	–3671(20)	24(22)	7.1(9)
C(24)	585(17)	–3022(15)	225(17)	4.6(6)

[a] Anisotropic thermal parameters ($\times 10^4$) in the form: $\exp[-(B_{11}h^2 + B_{12}hk + B_{13}hl + B_{22}k^2 + B_{23}kl + B_{33}l^2)$.

	B11	B12	B13	B22	B23	B33
I(1)	81(1)	36(2)	22(2)	43(1)	–8(2)	43(1)
I(2)	24(1)	2(1)	–4(1)	33(1)	15(1)	58(1)
Cu(1)	58(2)	25(3)	16(3)	38(1)	27(3)	44(1)
Cu(2)	41(1)	11(2)	4(3)	32(1)	10(2)	29(1)
P(1)	24(2)	2(5)	4(5)	31(2)	1(4)	29(3)
P(2)	27(2)	8(4)	–2(5)	23(2)	0(4)	30(3)

Solution and Refinement of the Structures

$(CuI)_2DPM$

The Patterson method was employed to locate the iodine atoms and Fourier methods to find the positions of all other non-hydrogen atoms. A full matrix isotropic refinement gave a conventional R index of 0.080. After the final least-squares refinement with anisotropic temperature factors for Cu, P and I atoms the R value was 0.056. The final weighting scheme was $w = 1/(A + B|F_o| + C|F_o|^2)$, where $A = 60.0$, $B = 1.0$ and $C = 0.0020$, chosen to maintain $w(|F_o| - |F_c|)^2$ essentially constant over all ranges of $|F_o|$ and $(\sin \Theta/\lambda)$. Table II presents the final values of the refined atomic parameters together with their standard deviations derived from the inverse matrix of the last least-squares refinement. No attempt was made to locate the hydrogen atoms.

TABLE III. Fractional Coordinates ($\times 10^4$) and Temperature Factors for the Two Independent Molecules of $(CuBr)_2$ DPM with their Estimated Standard Deviations in Parentheses.

	Molecule 1				Molecule 2			
	X	Y	Z	B	X	Y	Z	B
Br(1)	674(2)	1420(2)	1875(2)	a	5669(1)	3581(2)	4466(2)	a
Br(1)	−1073(1)	221(2)	−687(2)	a	3926(1)	4781(2)	3548(2)	a
Cu(1)	9(2)	287(2)	1475(2)	a	5006(2)	4713(2)	3548(2)	a
Cu(1)	−177(2)	−946(2)	−61(2)	a	4810(2)	5948(2)	4693(2)	a
P(1)	−150(4)	−552(4)	2234(5)	a	4822(3)	5550(4)	2447(5)	a
P(2)	−201(3)	−1764(4)	891(5)	a	4784(3)	6767(4)	3686(5)	a
CP	−683(12)	−1394(14)	1344(16)	2.7(5)	4318(11)	6417(14)	2322(16)	2.3(5)
C(1)	679(12)	−875(15)	3656(18)	3.1(7)	4138(13)	5202(16)	966(18)	3.4(6)
C(2)	1394(14)	−359(18)	4331(21)	4.9(8)	3301(13)	5414(16)	173(19)	4.0(7)
C(3)	2012(18)	−674(24)	5626(26)	7.7(11)	2740(14)	5057(18)	−904(20)	4.7(7)
C(4)	1989(18)	−1292(23)	5943(25)	7.2(10)	3047(13)	4547(15)	−1176(18)	3.4(6)
C(5)	1339(14)	−1781(19)	5220(20)	5.0(8)	3866(17)	4391(21)	−383(23)	6.1(9)
C(6)	649(13)	−1534(16)	4038(18)	3.6(6)	4439(13)	4750(17)	737(19)	4.1(6)
C(7)	−877(11)	−205(14)	2236(16)	2.7(5)	5690(13)	5878(16)	2658(18)	3.4(6)
C(8)	−586(13)	282(16)	3104(18)	3.8(6)	5640(14)	6517(17)	2265(20)	4.4(7)
C(9)	−1106(16)	590(21)	3136(23)	6.0(9)	6347(16)	6737(20)	2482(23)	6.0(9)
C(10)	−1995(14)	464(17)	2196(20)	4.4(7)	7027(16)	6183(21)	3163(23)	6.3(9)
C(11)	−2248(14)	−29(18)	1421(20)	4.9(8)	7024(17)	5577(21)	3552(24)	6.6(9)
C(12)	−1750(13)	−343(15)	1319(18)	3.8(6)	6390(15)	5368(18)	3362(21)	4.6(7)
C(13)	756(11)	−2221(13)	2189(15)	2.1(5)	4175(12)	7592(14)	3312(16)	2.8(9)
C(14)	1478(15)	−1919(19)	2538(21)	5.2(8)	4403(13)	8018(17)	4188(19)	4.1(7)
C(15)	2191(15)	−2329(19)	3544(21)	4.9(8)	3905(13)	8654(17)	3894(19)	4.0(6)
C(16)	2164(13)	−2887(16)	4086(18)	3.8(6)	3248(15)	8833(18)	2828(20)	4.8(7)
C(17)	1473(14)	−3124(18)	3640(20)	4.3(7)	2984(17)	8351(22)	1936(25)	7.0(10)
C(18)	748(12)	−2799(15)	2711(17)	3.2(6)	3450(13)	7748(17)	2141(19)	4.1(7)
C(19)	−818(11)	−2574(13)	57(15)	2.1(5)	5725(12)	7224(14)	4323(16)	2.5(5)
C(20)	−1548(13)	−2757(16)	−271(19)	3.8(7)	6445(14)	6997(18)	5400(20)	4.8(7)
C(21)	−2013(14)	−3401(17)	−959(20)	4.3(7)	7249(10)	7330(20)	5930(22)	5.7(9)
C(22)	−1829(15)	−3826(19)	−1374(22)	5.4(−0)	7214(15)	7841(19)	5295(21)	5.2(8)
C(23)	−1069(13)	−3652(17)	−1017(19)	4.0(6)	6454(15)	8118(19)	4244(21)	5.4(8)
C(24)	−622(13)	−2994(16)	−365(18)	3.9(6)	5720(13)	7753(15)	3728(18)	3.4(6)

[a] Anisotropic thermal parameters ($\times 10^4$) in the form: $\exp[-(B_{11}h^2 + B_{12}hk + B_{13}hl + B_{22}k^2 + B_{23}kl + B_{33}l^2)$

	B11	B12	B13	B22	B23	B33	B11	B12	B13	B22	B23	B33
Br(1)	50(1)	−35(2)	79(2)	34(1)	−35(2)	70(2)	53(1)	33(2)	115(2)	34(1)	34(2)	98(2)
Br(1)	20(1)	2(1)	39(1)	28(1)	12(2)	63(2)	20(1)	0(2)	30(1)	27(1)	6(2)	54(2)
Cu(1)	35(1)	−3(2)	77(2)	29(1)	5(3)	78(2)	43(1)	4(2)	68(2)	26(1)	14(3)	62(2)
Cu(1)	33(1)	−1(2)	57(2)	26(1)	2(2)	56(2)	34(1)	7(2)	62(2)	27(1)	16(3)	60(2)
P(1)	19(2)	−8(4)	31(4)	22(2)	−9(5)	48(4)	25(2)	9(4)	43(4)	25(2)	7(5)	42(4)
P(2)	20(2)	1(3)	43(3)	20(2)	0(5)	44(3)	21(2)	7(3)	31(3)	21(2)	−1(5)	31(3)

TABLE IV. (CuI)$_2$DPM – Absolute Values of Observed and Calculated Structure Factors (× 10).

K	L	FO	FC
*00*00H*			0*0000
0	4	3356	3216
0	6	4339	4215
0	8	5575	5308
0	10	1294	474
0	12	2080	1925
0	14	1126	1088
0	16	656	496
0	18	688	681
2	3	3105	3114
2	4	3802	3746
2	5	1674	1791
2	6	1785	1592
2	7	556	513
2	8	485	446
2	9	2620	2576
2	10	1223	1098
2	12	854	782
2	13	1650	1610
2	17	685	631
4	0	2132	1740
4	1	1728	1790
4	2	592	653
4	3	3885	3678
4	5	640	726
4	6	947	920
4	8	1690	1757
4	10	924	950
4	12	1171	1141
4	13	690	481
4	14	1438	1302
4	16	830	725
6	0	5192	5303
6	1	651	650
6	2	762	848
6	3	1258	1143
6	4	3646	3838
6	5	1916	2113
6	6	642	597
6	7	2071	2122
6	8	1299	1255
6	10	1379	1394
6	11	667	664
6	12	2262	2242
6	14	650	660
8	0	3018	2860
8	1	2181	2241
8	2	2325	2232
8	3	3719	3700
8	4	602	479
8	5	865	961
8	6	2291	2401
8	8	1015	1013
8	9	3553	3598
8	10	656	760
8	12	729	806
8	13	1030	1020
8	17	686	640
10	0	948	203
10	1	2246	2157
10	2	2578	2581
10	3	2312	2410
10	4	2767	2773
10	5	569	522
10	6	987	1018
10	7	533	648
10	9	2077	2049
10	10	1517	1595
10	11	698	708
12	0	532	402
12	2	755	765
12	5	1977	1932
12	7	1319	1321
12	8	746	719
12	9	894	1051
12	10	574	543
14	1	1112	1084
14	2	994	1110
14	3	1006	1160
14	4	833	905
14	9	1266	1300
14	10	694	823
16	0	1152	1058
16	1	1169	1112
16	3	1018	1127
16	6	1133	1068
16	9	1412	1463
18	1	883	751
18	5	719	706
18	7	706	772
*00*00H*			1*0000
0	4	2970	2856
0	6	2794	2719
0	8	1102	1008
0	10	740	640
0	12	1193	1146
0	14	658	602
1	3	1518	1198
1	4	1208	1250
1	5	780	713
1	6	1923	1951
1	7	4095	4077
1	8	1976	1837
1	9	1807	1701
1	11	1866	1806
1	12	1227	1242
1	14	765	711
2	3	2989	2871
2	5	511	541
2	6	2012	1848
2	7	576	788
2	8	1651	1559
2	10	1226	1198
3	2	3672	3734
3	3	3510	3667
3	4	665	631
3	5	2047	2043
3	6	1316	1375
3	7	689	820
3	8	1172	1138
3	9	807	787
3	10	601	619
3	11	669	672
3	14	752	703
3	15	1085	1040
4	4	1461	1422
4	5	950	953
4	6	684	649
4	8	1459	1462
4	10	1081	1097
4	13	553	480
5	1	1107	1067
5	2	1742	1808
5	3	569	506
5	4	1012	1142
5	5	2425	2331
5	9	769	747
5	10	539	447
5	11	1593	1546
5	12	1495	1524
5	13	1500	1441
5	15	846	784
6	1	1744	1853
6	4	1438	1386
6	6	1536	1546
6	7	1017	1254
6	8	595	597
6	11	722	728
6	12	756	754
7	1	3132	2994
7	2	1743	1814
7	3	1708	1731
7	5	726	832
7	7	1623	1768
7	8	2199	2279
7	10	912	953
7	11	1485	1597
7	13	794	792
7	15	633	644
7	16	681	641
7	17	664	669
8	3	1916	1885
8	4	1033	1119
8	5	1641	1664
8	6	1407	1563
8	7	642	658
9	1	1425	1323
9	2	3876	3876
9	3	2225	2319
9	5	1189	1266
9	6	853	886
9	7	1046	1101
9	8	1917	1962
9	10	2048	2165
9	11	753	699
10	1	1402	1448
10	3	1149	1107
10	4	555	511
10	5	669	724
10	8	643	669
11	1	1136	1068
11	2	496	469
11	3	2158	2266
11	4	831	817
11	6	1352	1310
11	9	742	788
11	11	1497	1485
12	1	1361	1384
13	3	706	552
13	6	1318	1347
13	7	553	477
13	10	673	664
13	11	696	666
14	1	814	817
14	2	666	686
14	3	640	503
15	1	735	740
15	2	2016	1936
15	3	1012	983
15	10	1075	1072
16	3	949	901
17	1	858	785
17	7	794	862
18	1	677	629
*00*00H*			2*0000
0	4	790	548
0	6	2538	2398
0	8	4295	4037
0	14	1267	1234
0	16	703	648
1	3	897	795
1	4	1087	1292
1	5	4472	4366
1	6	762	665
1	7	3107	3015
1	8	1529	1484
1	11	948	909
1	13	1192	1140
1	14	662	550
2	2	830	369
2	3	1829	1764
2	4	501	624
2	5	2797	2855
2	6	546	714
2	8	1315	1322
2	9	1621	1617
2	13	1302	1245
3	0	480	194
3	1	3565	3644
3	2	1436	1437
3	3	5027	4920
3	4	769	821
3	6	972	997
3	7	1465	1482
3	8	898	968
3	9	3195	3228
3	11	1075	995
4	0	1532	1402
4	2	542	543
4	3	1523	1517
4	4	1120	1027
4	5	1332	1180
4	6	1744	1721
4	8	875	939
4	9	509	579
4	10	671	720
4	12	820	826
4	14	828	821
5	0	5050	4998
5	1	1291	1297
5	2	1883	1755
5	3	496	659
5	4	582	738
5	5	1789	1889
5	6	840	1126
5	7	2213	2218
5	8	872	966
5	9	1044	1042
5	10	994	1071
5	11	807	797
5	12	1162	1168
6	0	1924	1848
6	1	434	508
6	2	849	854
6	3	567	486
6	4	3965	4188
6	7	1091	1055
6	8	561	570
6	10	1031	1180
6	12	1486	1466
7	0	2934	2683
7	1	933	934
7	2	2600	2582
7	4	1390	1650
7	5	2323	2392
7	7	1559	1637
7	11	768	718
7	13	865	913
8	0	1018	934
8	1	1728	1748
8	2	634	542
8	3	1406	1302
8	4	778	782
8	5	1724	1729
8	6	1440	1435
8	9	1924	1958
8	13	948	951
8	17	679	610
9	2	2551	2605
9	4	2501	2625
9	7	878	837
9	8	712	725
9	9	854	842
9	14	855	913
10	1	1789	1690
10	2	2058	1954
10	3	1098	1113
10	4	1504	1548
10	5	695	703
10	6	653	719
10	7	738	787
10	9	830	937
10	10	1428	1393
10	12	607	532
11	0	2422	2457
11	1	882	809
11	2	1355	1341
11	3	854	879
11	5	731	702
11	9	1192	1277
11	12	739	762
12	0	837	747
12	3	555	586
12	5	526	444
13	0	1752	1753
13	1	908	828
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9	0	2523	2390
9	1	621	505
9	2	1159	1119
9	5	656	694
9	6	638	624
9	7	964	953
10	0	821	800
10	1	952	846
10	2	671	700
10	6	793	817
10	9	674	672
11	2	632	542
11	4	1187	1164
11	5	634	683
12	1	730	653
12	9	820	864
13	4	833	906
13	8	623	624
15	0	857	904
17	0	758	771
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0	4	1102	1202
0	6	893	984
0	8	1222	1176
0	10	1298	1474
1	1	657	642
1	3	528	598
1	9	694	707
2	3	908	1000
2	4	1090	1191
2	6	2222	2476
2	8	1164	1187
2	9	713	776
2	11	920	923
3	3	603	705
3	6	620	684
4	2	694	663
4	3	912	921
4	4	947	960
4	6	2418	2578
4	7	612	653
4	12	753	757
5	3	592	707
5	6	606	647
6	2	1154	1080
6	3	2188	2174
6	4	931	990
6	5	844	892
6	10	606	616
7	5	640	625
8	1	2284	2147
8	3	1231	1224
8	5	687	757
8	6	816	746
8	7	1120	1082
8	8	1068	1108
9	6	645	691
9	7	651	628
10	1	1320	1270
10	3	1121	1087
10	4	637	601
10	6	844	851
10	12	692	648
11	2	654	597
12	3	1153	1147
12	7	760	766
14	1	690	701
16	1	954	950
18	3	778	884
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0	4	1016	961
0	8	686	638
0	14	751	613
1	0	527	406
1	1	591	612
1	3	803	803
1	5	1141	1242
1	7	764	733
1	9	867	998
1	10	657	751
2	0	836	790
2	2	1402	1413
2	5	772	738
3	b	625	162
3	1	689	655
3	4	713	841
3	5	1918	2020
3	7	1259	1304
4	0	1551	1434
4	2	1315	1279
4	4	823	902
4	5	807	809
5	2	1217	1152
5	3	945	979
5	4	628	584
5	5	772	777
6	0	1173	1051
6	2	890	828
6	4	1325	1227
7	0	949	824
7	2	1346	1332
7	4	1247	1315
7	6	917	978
7	7	682	676
8	4	733	681
8	5	926	897
8	7	712	720
9	0	1802	1796
9	1	750	609
9	2	805	771
9	7	634	766
10	0	776	684
10	1	578	438
10	5	792	765
10	7	824	824
11	0	597	207
11	4	905	862
13	4	725	681
15	0	929	864
*00*00H*			13*0000
1	1	900	938
1	3	1666	1714
1	5	1075	1084
1	13	695	737
2	1	577	522
2	2	747	672
2	3	770	795
2	6	645	694
2	9	644	751
3	1	2023	1826
3	2	620	482
3	3	1183	1208
3	6	795	834
4	5	583	632
5	1	1378	1344
5	2	873	776
5	3	1325	1265
5	5	1026	1088
5	10	670	659
7	3	1186	1135
7	4	680	698
7	5	765	772
7	6	987	1050
8	1	582	511
9	1	656	527
9	4	948	959
9	6	1296	1293
11	4	767	776
11	6	631	640
12	1	645	629
13	8	692	693
*00*00H*			14*0000
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0	4	1395	1379
0	8	694	710
1	0	887	762
1	3	639	696
1	9	644	603
2	0	1499	1331
2	2	1329	1367
2	5	698	725
3	0	1370	1167
3	3	1121	1150
3	4	710	814
3	9	708	741
4	0	1204	1104
4	2	1022	1012
4	4	621	570
4	5	601	660
5	0	973	886
6	0	735	653
6	2	815	763
6	4	1090	1027
8	4	761	763
8	5	1025	977
8	7	760	760
9	1	695	700
9	3	605	387
10	0	726	623
10	5	705	725
10	7	675	680
11	0	984	910
13	0	914	886
13	2	758	835
*00*00H*			15*0000
0	2	780	610
0	6	678	848
0	8	1126	1302
2	1	1218	1132
2	2	732	819
2	4	1002	1008
2	8	742	847
4	1	737	676
4	2	596	620
4	3	661	634
4	5	745	725
4	8	802	860
6	6	806	849
8	1	799	689
8	2	718	725
10	1	619	688
12	1	1041	1185
12	3	749	729
14	3	662	669
*00*00H*			16*0000
1	0	684	605
1	3	839	976
1	9	683	722
2	0	826	706
3	0	1008	1011
3	3	689	849
3	5	805	738
3	7	661	636
5	0	609	726
5	4	737	661
5	9	726	769
6	0	669	611
7	0	956	871
9	0	876	840
11	0	670	706
11	2	683	722
13	0	915	896
13	2	730	859
*00*00H*			17*0000
1	1	1168	1125
1	5	652	588
2	1	817	743
*00*00H*			18*0000
0	0	966	912
0	2	691	758
0	4	678	770
1	0	704	538
2	0	1196	1117
2	2	716	735
4	0	981	798
4	2	776	727

TABLE V. (CuBr)$_2$DPM – Absolute Values (× 10) of Observed and Calculated Structure Factors.

K	L	FO	FC
*00*00H*			0*0000
0	4	1372	1280
0	6	701	685
0	8	511	523
0	10	1029	1054
1	3	2546	2391
1	4	1079	1107
1	5	1329	1269
1	6	609	487
1	7	1457	1456
1	8	393	510
1	9	815	807
1	11	769	830
1	13	592	616
2	2	846	595
2	3	2693	2435
2	4	1791	1606
2	6	1063	980
2	7	1029	989
2	8	603	585
2	9	638	478
2	10	1293	1190
2	11	582	601
3	2	1125	907
3	3	2220	1975
3	4	629	396
3	5	1103	1088
3	6	755	642
3	7	1459	1349
3	11	832	871
3	12	772	836
3	13	888	791
4		1197	1211
4	1	266	178
4	2	1063	962
4	3	811	681
4	4	3034	2765
4	5	1822	1667
4	9	577	471
4	1	1147	1084
4	13	793	660
5	2	1825	1642
5	3	4107	4005
5	4	1760	1593
5	5	2578	2263
5	9	619	535
5	11	758	725
5	13	566	537
6		2676	2630
6	1	1313	1254
6	2	920	936
6	4	3684	3331
6	6	1166	751
6	7	746	598
6	8	785	782
6	1	553	556
7	1	1697	1696
7	2	2156	2018
7	3	1524	1398
7	4	393	388
7	6	1033	832
7	7	683	228
7	9	1276	1262
8		1230	1060
8	1	366	363
8	2	699	615
8	3	2690	2598
8	4	765	686
8	5	1371	1390
8	6	633	706
8	8	839	846
9	1	630	661
9	2	1772	1706
9	3	1267	1165
9	4	1778	1657
9	5	597	[illegible]
9	6	675	196
9	8	951	781
9	10	569	635
9	12	750	763
10		868	821
10	1	1115	1161
10	2	1866	1799
10	3	1330	1398
10	4	506	495
10	8	756	621
10	9	1095	1056
11	1	531	629
11	2	931	925
11	3	1371	1328
11	6	579	646
11	7	860	839
11	9	606	687
12		819	723
12	1	919	965
12	2	959	931
12	11	596	629
13	2	737	686
13	4	519	633
13	6	639	558
13	7	708	716
13	1	835	746
14		676	697
14	1	662	706
14	4	751	658
14	5	525	593
14	6	670	676
15	1	1069	1035
15	2	536	505
15	7	679	633
16		1497	1532
16	2	621	589
16	3	767	867
16	6	665	632
17	1	1129	1148
17	2	471	460
17	4	588	558
17	9	605	515
18		1258	1183
18	4	530	526
19	1	572	537
19	3	522	539
20	4	856	815
*00*00H*			1*0000
0	2	662	624
0	-4	1303	1462
0	6	1192	1085
0	-6	2052	2067
0	8	606	601
0	-8	1066	1056
0	10	2038	2215
0	-10	1137	1167
0	-12	865	855
1	2	823	691
1	3	315	160
1	-3	605	665
1	4	892	808
1	-4	652	605
1	5	601	380
1	-5	1732	1813
1	6	1091	1043
1	-6	330	308
1	7	1554	1521
1	-7	1139	1023
1	9	1431	1390
1	11	738	836
1	-11	762	737
2	2	559	573
2	3	783	733
2	-3	1331	1389
2	4	749	626
2	-4	1165	1152
2	5	671	679
2	-5	1966	1977
2	6	1102	986
2	-6	381	326
2	7	1402	1499
2	-7	1109	1167
2	8	451	404
2	-8	1127	1079
2	-9	636	735
2	10	728	671
2	-11	665	380
3	1	2703	2571
3	-2	2421	3450
3	3	944	839
3	-3	3626	4348
3	4	1648	1536
3	5	1426	1436
3	-5	377	290
3	6	411	446
3	-6	1870	1905
3	7	525	494
3	-7	1565	1532
3	8	755	772
3	-9	524	576
3	-11	638	643
4	1	1100	868
4	-1	767	791
4	2	2783	2562
4	-2	629	601
4	-3	1067	1275
4	4	749	788
4	-4	2295	2634
4	5	2326	2212
4	-5	2590	2791
4	6	1769	1678
4	-6	1268	1296
4	-7	836	879
4	-8	972	1103
4	9	476	523
4	-9	409	317
4	-10	638	735
5	1	1127	1133
5	2	779	763
5	-2	472	445
5	3	499	549
5	-3	351	425
5	4	982	931
5	5	1778	1667
5	6	2245	2129
5	-6	2761	3066
5	7	1319	1298
5	-7	1578	1656
5	8	1285	1313
5	-8	661	339
5	-9	883	970
5	-10	903	999
6	1	291	207
6	2	376	331
6	3	342	286
6	-3	569	511
6	4	507	562
6	-4	566	638
6	5	2741	2676
6	-5	2229	2555
6	6	1666	1296
6	-7	962	869
6	8	868	866
6	-8	1179	1337
6	9	769	750
6	-9	1326	1330
7	1	496	418
7	2	429	507
7	-2	1532	1729
7	3	876	863
7	4	1661	1583
7	-4	531	569
7	5	492	499
7	-5	1395	1293
7	6	583	318
7	-6	1169	1256
7	7	769	818
7	8	1750	1667
7	-8	1066	1177
7	-9	930	890
7	-10	620	651
8	1	1563	1519
8	-1	1620	1399
8	2	659	609
8	-3	1368	1431
8	-4	423	417
8	5	1003	962
8	-5	1624	2010
8	6	611	332
8	-6	519	570
8	7	1966	1959
8	-7	728	801
8	9	968	912
8	-9	757	756
9	2	1580	1497
9	-2	3306	3521
9	4	1458	1368
9	5	558	593
9	6	662	515
9	-6	937	1069
9	8	1626	1288
9	-8	482	516
10	1	2009	1965
10	-1	2205	2251
10	2	1101	1053
10	3	801	630
10	-3	1251	1405
10	4	606	602
10	-4	686	525
10	5	1263	1218
10	-5	1458	1562
10	-6	608	635
10	7	662	581
10	8	550	520
10	9	999	908
10	-9	850	927
11	1	560	582
11	2	557	682
11	-2	956	1068
11	3	1456	1449
11	-3	895	920
11	4	1409	1303
11	-4	868	832
11	5	576	599
11	-5	677	560
11	6	676	586
11	-6	1626	1438
11	7	656	432
11	8	886	956
11	-10	890	912
11	11	565	568
12	2	643	712
12	-2	660	417
12	3	755	736
12	-3	688	711
12	5	1076	974
12	-5	1205	1367
12	-7	919	1014
12	9	995	976
12	-9	734	758
13	1	578	496
13	3	566	579
13	-3	668	515
13	4	1176	1109
13	-4	1069	1130
13	5	538	524
13	6	1133	1115
13	-6	1288	1462
13	-7	669	650
13	8	695	638
14	1	637	567
14	-1	659	648
14	2	1093	1098
14	-2	554	580
14	3	752	795
14	-4	613	586
14	5	929	961
14	-5	768	906
14	6	582	535
14	-6	781	763
14	-7	683	746
14	-9	503	546
15	2	553	641
15	-2	1279	1310
15	3	661	692
15	-3	636	647
15	4	619	579
15	-4	491	543
15	-6	749	833
16	1	746	696
16	-1	902	915
16	-3	662	666
17	-2	480	527
19	-2	532	568
20	6	588	618
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0	-4	558	366
0	6	869	892
0	-6	1658	1551
0	-8	1595	1666
0	-10	1136	1196
1	1	4069	4016
1	2	939	885
1	3	1500	1466
1	-4	635	519
1	5	942	979
1	-5	568	519
1	6	714	610
1	-6	612	508
1	7	574	686
1	-7	1667	1730
1	-8	1155	1223
1	-11	995	1033
1	-12	621	556
2	1	2091	1893
2	2	2056	1986
2	3	1014	933
2	-3	1777	2005
2	4	837	713
2	-4	540	706
2	5	713	686
2	-5	1022	1025
2	6	923	952
2	-6	657	677
2	-7	1161	1177
2	-8	981	1011
2	-9	949	976
2	-10	1167	1192
2	11	523	476
2	-12	513	469
2	-13	725	719
3	0	398	209
3	1	1759	1659
3	-2	419	141
3	3	3766	3561
3	4	1453	1313
3	5	956	1029
3	-5	755	655
3	-6	613	437
3	7	758	800
3	-7	661	785
3	8	662	658
3	-8	503	569
3	10	476	323
3	-11	1248	1240
3	-12	921	910
4	0	1241	1159
4	1	1161	1047
4	-1	324	156
4	2	2876	2510
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4	3	1662	1532
4	4	2730	2761
4	-4	525	591
4	5	1676	1331
4	-5	1103	1200
4	-8	859	955
4	9	487	446
4	-10	944	947
4	12	665	656
4	-12	737	710
4	-13	839	798
5	0	3672	3650
5	1	1757	1627
5	2	142	249
5	3	1668	1692
5	-3	1163	1161
5	4	2717	2653
5	-4	599	562
5	5	1691	1276
5	-5	1660	1829
5	8	916	926
5	-8	885	688
5	-10	607	595
5	-11	1006	1068
6	0	763	721
6	1	2730	2706
6	-1	1267	1316
6	2	1918	1819
6	-2	279	165
6	4	1897	1768
6	-4	2924	3410
6	-6	826	850
6	-7	556	631
6	8	579	598
6	-8	695	616
6	9	726	765
6	-9	617	626
6	-10	586	583
7	0	2577	2567
7	1	351	353
7	-1	1570	1526
7	2	1352	1239
7	3	1121	1118
7	-3	1662	1630
7	4	635	446
7	-4	616	781
7	-5	1193	1368
7	6	973	989
7	-6	568	604
7	-9	1110	1135
7	-10	625	615
8	1	523	460
8	-1	537	155
8	2	383	302
8	-2	1393	1445
8	3	1151	1125
8	-3	1056	1193
8	4	646	593
8	-4	523	665
8	5	618	530
8	-5	1792	1908
8	6	813	796
8	-6	408	387
8	7	913	852
8	-8	705	846
8	-9	502	595
9	-1	603	583
9	2	1136	1125
9	3	569	556
9	-3	1314	1529
9	-4	1608	1798
9	5	684	709
9	-5	810	986
9	-6	613	656
9	8	692	617
9	-8	519	612
9	-10	1020	1098
9	-12	571	579
10	1	1367	1367
10	-1	1103	1119
10	2	1358	1367
10	-2	1689	1890
10	-3	675	700
10	-4	1433	1534
10	5	501	481
10	-5	646	671
10	-6	770	868
10	-8	643	810
10	-9	813	921
10	-10	614	662
10	-13	603	671
11	0	1493	1557
11	1	438	456
11	-1	668	614
11	2	401	421
11	3	462	366
11	-3	1926	2068
11	4	1108	1043
11	6	449	356
11	-6	400	362
11	-7	436	421
11	-8	436	567
11	-9	970	1027
12	1	1383	1313
12	-1	952	906
12	2	1016	987
12	-2	910	948
12	4	1011	1078
12	-4	610	553
12	5	514	521
12	-8	439	456
12	9	878	899
13	0	1228	1355
13	3	806	786
13	4	595	534
13	5	578	615
13	6	536	480
13	-7	650	657
13	8	697	668
13	10	800	844
14	0	684	665
14	1	442	362
14	-1	628	619
14	-2	624	663
14	4	988	967
14	-6	666	689
14	-8	768	815
15	0	462	406
15	1	852	855
15	-1	1007	1052
15	3	751	765
15	-3	700	810
15	-4	631	643
15	7	699	582
15	-7	871	963
16	0	1084	1127
16	-2	688	658
16	-3	668	556
16	-5	667	675
16	6	620	568
16	-6	717	795
17	-1	1127	1103
17	-4	607	536
17	5	634	518
17	-7	662	737
18	0	790	815
18	-2	558	604
18	-4	593	585
18	-8	561	523
19	0	555	599
19	-1	569	550
19	3	685	614
20	6	739	761
21	-6	662	651
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0	-4	2011	2056
0	6	716	716
0	-6	4015	4209
0	8	565	626
0	-8	598	526
0	10	1608	1666
0	-12	736	743
1	2	1390	1368
1	3	1662	1527
1	4	586	553
1	-4	588	622
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TABLE V. (Cont.)

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8	-8	441	340
8	-9	899	1045
9	0	1926	2005
9	2	490	365
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9	-3	742	644
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9	-8	409	386
9	-10	1070	1127
10	1	1026	961
10	-1	1445	1472
10	-4	580	653
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11	0	593	513
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11	-7	405	395
11	-9	662	647
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13	-5	576	595
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*00*00H*		13*0000	
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7	-9	763	776
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9	-8	853	752
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6	-10	841	872
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10	-5	534	552
10	-6	514	563
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10	-9	859	886
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11	-4	558	628
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11	-8	804	908
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2	-10	1029	1108
3	0	587	768
3	1	772	886
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3	-6	508	543
3	-7	573	585
3	-8	652	589
4	0	816	742
4	-4	462	444
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4	-10	899	950
5	-3	597	553
5	-8	888	788
5	-9	477	504
5	-10	578	488
6	-4	667	678
6	-5	501	521
6	-8	596	444
6	-10	560	570
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7	-9	1089	1148
7	-10	602	570
8	-1	537	626
8	-4	728	780
8	-5	488	445
8	-7	917	943
9	-10	974	1047
10	-9	920	984
10	-10	949	569
11	-9	527	641
12	-7	586	625
12	-10	478	398
13	-2	742	844
13	-8	568	587
14	-7	516	484

(CuBr)$_2$DPM

Examination of the Patterson map allowed the location of the eight independent copper and bromide atoms. The remaining atoms were located following successive structure factor and Fourier calculations. Isotropic temperature factors and positional parameters of all non-hydrogen atoms were refined by a block diagonal least-squares method to a R value of 0.10. At this point anisotropic temperature factors were assigned to the Cu, Br and P atoms. Subsequent refinement resulted in the R value of 0.074. The final weighting scheme was as in the above case with A = 30.0, B = 1.0 and C = 0.0030. Table III lists the values of the final atomic parameters together with their standard deviations calculated as described above. No attempt was made to locate hydrogen atoms. All calculations were carried out on a CDC6200 computer using programs described in refs. 5, 6.

Observed and calculated structure factors are reported in Tables IV and V for (CuI)$_2$DPM and (CuBr)$_2$DPM respectively.

Results

Description of the Structures

Both the compounds may be described in terms of discrete tetranuclear units (CuX)$_4$DPM$_2$, strictly cen-

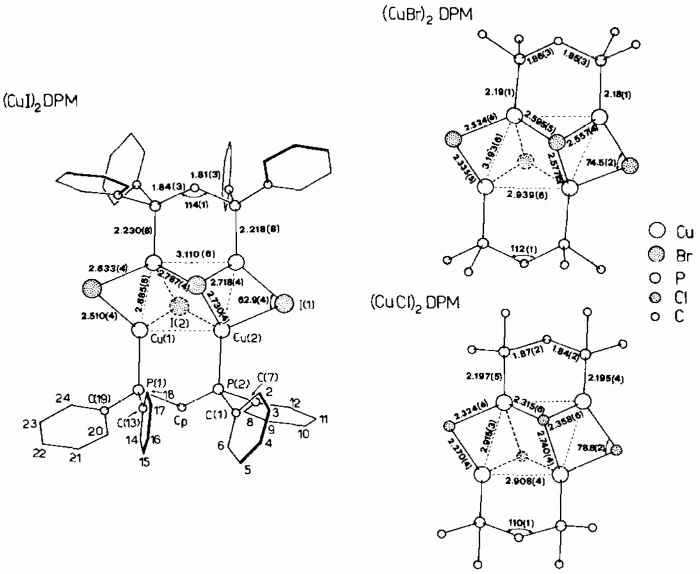


Figure 1. A comparison of the structures of the three complexes $(CuX)_2DPM$. Some bond lengths and angles of interest are reported. The numbering scheme for the atoms is reported for the iodine compound. The same numbering scheme is applied to each of the two independent $(CuBr)_2DPM$ molecules. The mean values of bond lengths and angles are reported for the bromine derivative.

trosymmetric, held together by efficient phenyl–phenyl interactions. The same geometry was found for the analogous chlorine derivative[3] with differences only in the fine details. A comparison of the three structures is shown in Figure 1, where some distances of interest are also reported. The bromine and iodine derivatives are quite similar, making allowances for the different sizes of the involved halogens, whereas the chlorine compound differs because one of the Cu–Cl distances involving the trico-ordinate Cl atom is greatly increased with respect to the others. This corresponds to the different conformation of the Cu–X–Cu–P–Cp–P ring, which has a chair-like conformation in the chlorine derivative and a boat-like conformation in the iodine and bromine compounds (Figure 1). Although the Cu–P bond lengths are uninfluenced by the different co-ordination of copper atoms in all these compounds, the Cu–X distances are significantly different. The distances involving the triple bridged Br and I atoms are systematically longer than those of the corresponding double bridged atoms. The double bridge is asymmetric, the two bond lengths being significantly different. The $(CuX)_4$ core may be described as an eight-membered ring with alternating Cu and X atoms; the third position on the copper atoms being occupied by a phosphorus atom. The ring assumes two conformations, depending on the ligand L. The centro-symmetric conformation $\bar{1}$ of Figure 2d, which may be called "step" conformation[9], is stabilized by bidentate ligands such as DPM, which force pairs of copper atoms to come on closer together. The cubane-type conformation (Figure 2e), of approximately $\bar{4}$ symmetry, on the contrary seems to be stabilized by bulky monodentate ligands. The two conformations also differ in the number of CuCl bonds, which can be formed: in the cubane structure there are three per Cu atom, whereas in the $\bar{1}$ conformation there are 2.5.

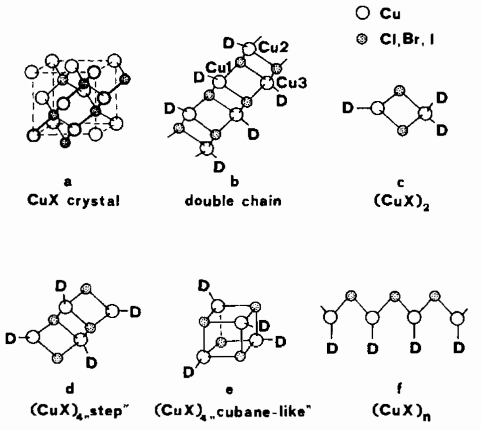


Figure 2. Comparison of all the known $(CuX)_n$ core structures.

TABLE VI. Structures of $(CuX)_n(D_x\text{–}L)_m$ Compounds.

Compound	Structure	a	Cu/D ratio	ref.
$(CuX)CH_3CN$ (X = Cl, Br)	double stranded chain	4	1/1	7
$(CuCl)CH_3N{=}NCH_3$	double stranded chain	4	1/2	8
$(CuX)\cdot PPh_3$ (X = Cl)	$\bar{4}$-$(CuCl)_4$ "cubane"	4	1/1	9
$(CuBr)\cdot PPh_3$	$\bar{1}$-$(CuBr)_4$ "step"	3.5	1/1	9
$(CuX)_2\cdot DPM$ (X = Cl, Br, I)	$\bar{1}$-$(CuX)_4$ "step"	3.5	1/1	3, present paper
$(CuCl)\cdot DPM$	$[Cu_3Cl_2DPM_3]^+$	4	1/2	10
$(CuCl)_2(PPh_3)_3$	dimer	3.5	2/3	11
$(CuI)\cdot nas^b$	dimer	4	1/2	12
$(CuCl)_2(DPE)_3$	dimer	4	1/3	13
$(CuCl)(PPh_3)_3$	monomer	4	1/3	14
$(CuCl)(dmt)_3$	monomer	4	1/3	15
$(CuCl)\cdot COTR$	single chain	3	1/1	16
$(CuCl)\cdot$ 1,6-heptadiyne	single chain	3	1/2	17
$(CuCl)\cdot$ norbornadiene	$\bar{4}$-$(CuCl)_4$	3	1/1	18
$(CuCl)\cdot$ 1,2-butyne	$\bar{4}$-$(CuCl)_4$	3	1/1	17
$(CuCl)_2(COT)_3$	dimer	3.5	2/3	19
$(CuCl)_2(COD)_2$	dimer	4	1/2	20
$(CuCl)\cdot Et_4P_2$	single chain	4	1/2	21
$(CuCl)\cdot Et_4S_2$	single chain	4	1/2	22

[a] Mean coordination number of copper atoms. [b] nas = (*o*-dimethylaminophenyl)dimethylarsine-*As*, *N*).

Discussion

The known structures of $(CuX)_n(D_x\text{–}L)_m$ compounds (X = Cl, Br, I; D = co-ordinated atom of a L ligand, x being 1 for mono- and 2 for bi-dentate ligands) are summarized in Table VI. The backbone structures of the $(CuX)_4$ core are sketched in Figure 2.

The experimental results may be summarized as follows: i) the degree of polymerization of the $(CuX)_n$ core depends upon the nature and size of the ligand and upon the stoichiometry of the compound; ii) the building up of polynuclear species is limited by the fact that the copper atom does not assume a co-ordination number higher than four. Consequently at least one Cu–Cl bond of the parent structure must be broken for each Cu–C bond formed; iii) the highest Cu/D ratio to have been observed is 1/3; iiii) most of the compounds were prepared directly starting from CuX and the ligand under suitable conditions.

On these grounds we propose a pictorial interpretation of the formation of the above structures starting from the same "basic" structure.

Brown and Dunitz[8] have already pointed out the resemblance of the double stranded infinite chains of Figure 2 (b)[7,8] with the infinite three-dimensional network of CuX itself (Figure 2(a)). We assume that the double chain is stabilized whichever L ligand is present. The copper atoms of the chain may undergo one, two or three attacks by the ligand, according to the reported stoichiometries.

When L is a monodentate ligand and three L molecules attack each copper atom of the double stranded chain, in agreement with the highest stoichiometry, a complete breakdown of the polymeric structure occurs with formation of tetrahedral mononuclear species, such as $CuCl(PPh_3)_3$[14] or $CuCl(dmt)_3$[15] (dmt = dimethylthiourea). This is due essentially to steric interactions of L with the chain. The formation of dinuclear species with 2/3 stoichiometry (Figure 3) may be explained in the same way, assuming that the copper atoms along the chain are alternately attacked by one and two ligand molecules. Compounds having structure such as $(CuCl)_2(PPh_3)_3$[11] and $(CuCl)_2(COT)_3$[19] (COT = *trans*-cyclooctene) are obtained.

In 1/1 stoichiometry, bulky phosphines, such as PPh_3, break-down the double chain as indicated in Figure 4, giving $(CuX)_4$ units (inspection of models shows that the arrangement of three ligand molecules on three adjacent copper atoms is sterically not possible). These

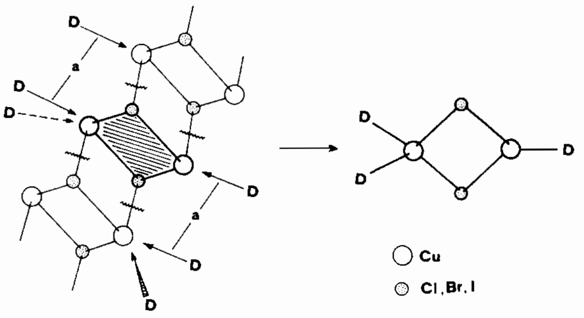


Figure 3. The steric hindrance in (a) between the ligands provokes the break-down of the Cu–X bonds as indicated.

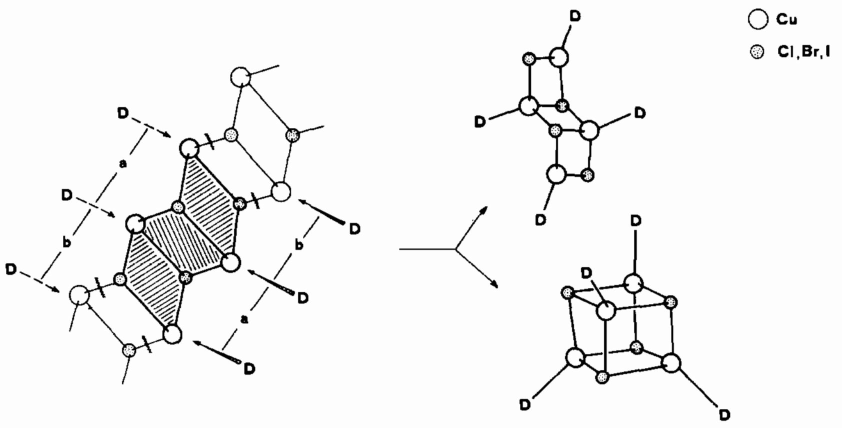
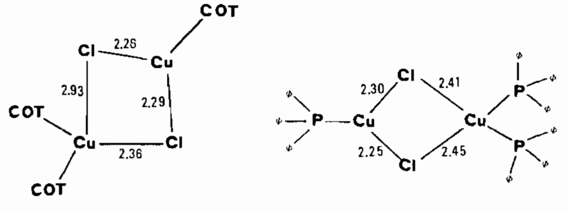


Figure 4. Ligand molecules, such as PPh_3 or DPM, may arrange with good Van der Waals contacts in (a). Correspondingly steric hindrance in (b) provokes the break-down of the Cu–X bonds in the way shown.

units may assume the "step" or cubane-like structure, as shown in Figure 4, probably depending upon a delicate balance of steric and electronic factors and crystal packing.

When L is a π-olefinic-like ligand the electronic influence due to the strong back-donation Cu → ligand favours the three-co-ordination of the copper atom. This suggestion appears to be confirmed by the comparison of the $(CuCl)_2(COT)_3$ and $(CuCl)_2(PPh_3)_3$ structures. In the former structure both copper atoms can be considered trigonal since the interaction with the Cl atom involved in the long Cu–Cl bond of 2.93 Å is very weak. The trigonal nature is also supported by the sum (359°) of the angles formed by the two COT molecules and the short-bonded Cl atom with the copper atom. On the contrary in $(CuCl)_2(PPh_3)_3$ one copper atom has a trigonal and the other a tetrahedral geometry.

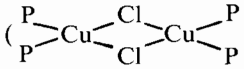


I

Thus, in 1/1 stoichiometry, infinite single chains $(-Cu-X-)_n$[16,17] or eight-membered $(CuCl)_4$ ring[17,18], in which the Cu atom was found to assume a trigonal geometry, may be obtained. The preferential formation of one of these kinds of structures depends mainly upon steric effects. Furthermore, when a cycloolefin can act as a bidentate ligand, for example 1,5-cyclooctadiene (COD), steric interactions provoke mainly the formation of dimeric species[20] in contrast with the polymeric structure of $[(CuCl)COTR]_n$[16], in which the COTR olefin acts as a monodentate ligand (COTR = cyclooctatetraene).

The 1/1 and 1/2 stoichiometries of compounds with non-bulky ligands having N-donor atoms, do not affect the main structure, that is the double-stranded chain is maintained[7,8].

As far as bidentate ligands are concerned, we wish to stress that, because of the variability of bond lengths and angles involving Cu and Cl atoms, it may be assumed that the double-stranded chain may fold or elongate such as an "accordion" along the chain direction or perpendicular to it. Looking at Figure 2, this means that the Cu1–Cu2 and Cu1–Cu3 distances may vary according to the bite of the ligand. It is to be noted that the former distance can vary more than the latter without altering substantially the double chain.

The DPM ligand, with its P···P bite of 3.1 Å attacks the CuX chain isolating $(CuX)_4$ units, as happens for the compounds with 1/1 Cu/P ratio formed by monodentate phosphine ligands (Figure 4). The bite value of DPM, however, allows only a distorted "step" geometry. On decreasing the Cu/P ratio the degree of polymerization is also compelled to decrease, because the co-ordination number of copper atoms cannot exceed four. The CuCl·DPM complex[10] has the structure shown in Figure 5. This unusual ionic structure, instead of forming a simple ( $\left(\begin{smallmatrix}P\\P\end{smallmatrix}{>}Cu{<}\begin{smallmatrix}Cl\\Cl\end{smallmatrix}{>}Cu{<}\begin{smallmatrix}P\\P\end{smallmatrix}\right)$) dimer, is justified by the difficulty of DPM in acting as chelating ligand. On the other hand less bulky diphosphines with a shorter P···P distance originate complexes with polymeric structure, for example $[CuX(C_2H_5)_4P_2]_n$ (X = Cl, Br)[21], suggesting that the attack of the bidentate ligand occurs on the Cu1 and Cu3

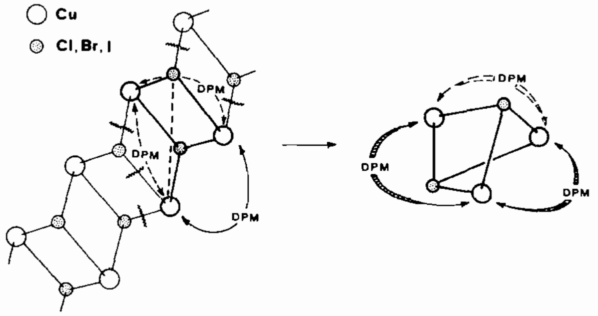


Figure 5. Formation of the $[Cu_3Cl_2(DPM)_3]^+$ ion.

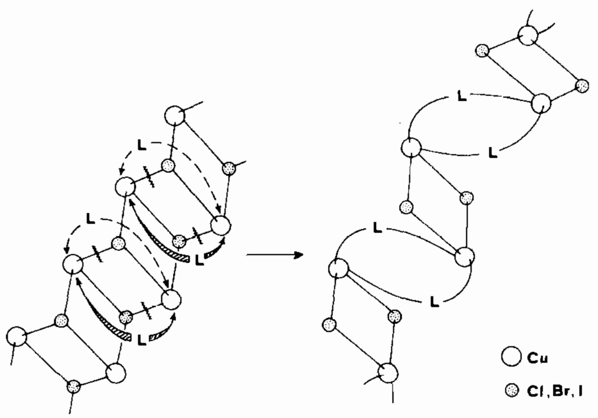


Figure 6. Formation of the polymeric double-bridged structure of $(CuX)_2Et_2P_2$.

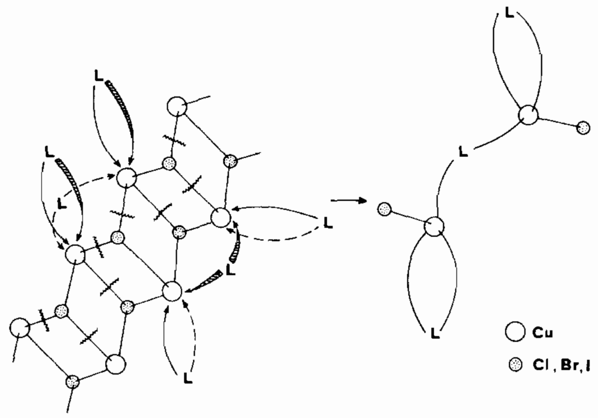


Figure 7. Formation of the $(CuCl)_2(DPE)_3$ dimeric species.

atoms, giving the chain shown in Figure 6. A slightly different polymeric chain may be originated in the same way for $CuCl(C_2H_5)_4S_2$[22].*

Finally, for a 1/3 Cu/P ratio, when the ligand may also act as chelate, as for example $Ph_2P(CH_2)_2PPh_2$ (DPE), dimeric units are formed[13] as shown in Figure 7, in contrast with the monomeric molecules obtained with the monodentate triphenylphosphine.

The above discussion suggests a preliminary rationalization of the known structures on the basis of rough steric effects. Obviously a more quantitative examination of steric as well as electronic effects is required to confirm this hypothesis.

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* It is to be noted, however, that the behaviour of sulphur containing ligands cannot be rationalized in the same way, because sulphur is able to co-ordinate one or more copper atoms in the same complex, giving compounds of identical stoichiometry but with different structures[23].