

Supporting Information

Mechanism of cytotoxicity of copper(I) complexes of 1,2-bis (diphenylphosphino) ethane

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Synthesis, ¹H, ³¹P NMR and elemental analysis data for the compounds used in the study

Synthesis, ^1H , ^{31}P NMR and elemental analysis data for the compounds used in the study

C1 was synthesized and characterized as previously described ¹.

$\text{Cu}_2(\text{DPPE})_3(\text{ClO}_4)_2$ (C2)

DPPE (0.2935 g, 0.735 mmol) was dissolved in 20 ml of CH_2Cl_2 and solid $\text{Cu}(\text{CH}_3\text{CN})_4\text{ClO}_4$ (0.1635 g, 0.5 mmol) was added. After 2 h of stirring, carbazole (0.0835 g, 0.5 mmol) was added followed by 24 h of stirring at room temperature. The complex was precipitated out by concentrating the solution to 5 ml and subsequent addition of diethyl ether (8 ml). The precipitate was washed four times with diethyl ether and dried in vacuo. The presence of carbazole was necessary to generate the complex C4. In the absence of carbazole, C1 was the major product formed. ^1H NMR (CDCl_3): δ 2.45(12H CH_2CH_2), 7.19, 7.3, 7.6, ^{31}P NMR (CDCl_3): δ -5.1, 5.1. IR (ν 1096 ClO_4).

$\text{Cu}(\text{DPPE})(\text{Benzotriazole})_2\text{ClO}_4$ (C3)

DPPE (0.199 g, 0.498 mmol) was dissolved in 20 ml of CH_2Cl_2 and solid $\text{Cu}(\text{CH}_3\text{CN})_4\text{ClO}_4$ (0.1635 g, 0.5 mmol) was added. After 2 h of stirring, benzotriazole (0.0595 g, 0.5 mmol) was added followed by 24 h of stirring at room temperature. The complex was isolated as above. ^1H NMR (CDCl_3): δ 2.43 (bs, 4H, CH_2CH_2), 7.6 (4H Bz), 7.3, 7.2. ^{31}P NMR (CDCl_3): δ -8.5 (s) 5.4(b).. IR (KBr pellet): 1099 (ν ClO_4).

$\text{Cu}_2(\text{DPPE})_3(\text{Benzotriazole})_2(\text{ClO}_4)_2$ (C4)

C4 was synthesized from $\text{Cu}(\text{CH}_3\text{CN})_4\text{ClO}_4$ using benzotriazole following the procedure used for synthesis of C3. Benzotriazole was however found coordinated to copper (I). ^1H NMR (CDCl_3): δ 2.445(bs, 4H, CH_2CH_2), 7.64, 7.3, 7.18. ^{31}P NMR (CDCl_3): δ -8.3 (s) – 4.7, 6.2 (b). IR (KBr pellet): 1090 (ν ClO_4).

Analytical Data in Tabular Form

Complex Formula	C		H		N	
	Calcd.	Found	Calcd.	Found	Calcd.	Found
C2 $C_{78}H_{48}Cu_2P_6Cl_2O_8$	55.63	55.36	H, 4.37	4.35		
C3 $C_{38}H_{34}N_6CuP_2ClO_4$	57.08	56.04	4.29	4.44	10.50	9.20
C4 $C_{90}H_{82}N_6P_6Cu_2Cl_2O_8$	59.26	59.35	4.59	4.73	4.55	3.41

Reference:

Vijayashree, N.; Samuelson, A.G.; Nethaji M.; 1,2-bis(diphenylphosphino)ethane(dppe) bridged dinuclear copper(I) complexes : Investigations of solid state and solution structures by CP/MAS ^{31}P NMR spectroscopy, X-ray crystallography, IR spectroscopy and solution ^{31}P and ^{65}Cu NMR spectroscopy. *Current Science*, **1993**, 65, 57-67.