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Crystal structure of (2,2'-bipyridine- κ^2N,N')bis(4-(dimethylamino)phenyldiphenylphosphane- κP) copper(I) tetrafluoroborate, $C_{50}H_{48}BCuF_4N_4P_2$

Table 1: Data collection and handling.

Crystal:	Plate, orange
Size:	0.54 × 0.40 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.61 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART APEX, ω -scans
$\theta_{\max}$, completeness:	50°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	45154, 5832, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4398
$N(\text{param})_{\text{refined}}$:	306
Programs:	Bruker programs [1], SHELX [2, 3], ORTEP-3 [4]

Source of material

The reaction of stoichiometric amounts, with the ratio (1/1/2) respectively of 2,2'-bipyridine, $[Cu(CH_3CN)_4]BF_4$ and 4-(dimethylamino)phenyldiphenylphosphine, in dichloromethane for 12 h followed by evaporation of the solvent yields a yellow powder. Re-crystallization from dimethylformamide affords crystals of the title compound.

Experimental details

All hydrogen atoms were placed in calculated positions using a riding model with C–H distances of 0.93 Å, or 0.96 Å. The isotropic displacement parameters were $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$ for the methyl atoms and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ for others.

Discussion

Heteroleptic copper(I) complexes based on diimine and phosphine ligands are of current interest owing to their chemical, photophysical and catalytic properties [5]. The reported structures of copper(I) complexes based on 4-(dimethylamino)phenyldiphenylphosphine are scarce in literature [6] and the structures of the corresponding heteroleptic complexes with 2,2'-bipyridine have not been reported to date.

The copper(I) ion is bonded to the two nitrogen atoms of 2,2'-bipyridine and the phosphorus atoms of two 4-(dimethylamino)phenyldiphenylphosphine molecules. The complex, including the copper(I) ion and the 2,2'-bipyridine ligand are located on a mirror plane. The geometry is distorted

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Abstract

$C_{50}H_{48}BCuF_4N_4P_2$, orthorhombic, $Pnma$ (no. 62), $a = 24.166(2)$ Å, $b = 19.5652(18)$ Å, $c = 9.6477(9)$ Å, $Z = 4$, $V = 4561.6(7)$ Å³, $R_{\text{gt}}(F) = 0.0494$, $wR_{\text{ref}}(F^2) = 0.1546$, $T = 298$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cu1	0.40157(2)	0.2500	0.26915(4)	0.03952(14)
N1	0.32491(12)	0.2500	0.3719(3)	0.0519(7)
N2	0.42698(13)	0.2500	0.4782(3)	0.0479(7)
N3	0.25946(13)	0.02825(15)	−0.2266(3)	0.0747(8)
P1	0.42314(2)	0.14640(3)	0.17719(6)	0.04038(16)
C1	0.27461(16)	0.2500	0.3161(5)	0.0634(10)
H1	0.2717	0.2500	0.2200	0.076*
C2	0.22640(17)	0.2500	0.3937(5)	0.0722(12)
H2	0.1920	0.2500	0.3507	0.087*
C3	0.23060(19)	0.2500	0.5343(6)	0.0758(13)
H3	0.1989	0.2500	0.5890	0.091*
C4	0.28144(19)	0.2500	0.5943(5)	0.0681(11)
H4	0.2847	0.2500	0.6903	0.082*
C5	0.32844(16)	0.2500	0.5123(4)	0.0508(8)
C6	0.38523(17)	0.2500	0.5694(4)	0.0522(8)
C7	0.3957(2)	0.2500	0.7123(4)	0.0719(13)
H7	0.3663	0.2500	0.7747	0.086*
C8	0.4487(3)	0.2500	0.7601(5)	0.0829(15)
H8	0.4558	0.2500	0.8548	0.099*
C9	0.4917(2)	0.2500	0.6664(5)	0.0753(13)
H9	0.5283	0.2500	0.6962	0.090*
C10	0.47881(17)	0.2500	0.5262(4)	0.0592(9)
H10	0.5077	0.2500	0.4625	0.071*
C11	0.37850(10)	0.11208(11)	0.0433(2)	0.0424(5)
C12	0.33199(10)	0.14860(12)	0.0017(3)	0.0468(5)
H12	0.3269	0.1925	0.0362	0.056*
C13	0.29335(11)	0.12261(13)	−0.0881(3)	0.0520(6)
H13	0.2632	0.1493	−0.1140	0.062*
C14	0.29873(11)	0.05655(14)	−0.1410(2)	0.0520(6)
C15	0.34625(12)	0.01979(14)	−0.1030(3)	0.0585(7)
H15	0.3520	−0.0236	−0.1398	0.070*
C16	0.38461(12)	0.04667(13)	−0.0122(3)	0.0529(6)
H16	0.4152	0.0206	0.0126	0.064*
C17	0.21112(18)	0.0668(2)	−0.2656(5)	0.0991(14)
H17A	0.1902	0.0781	−0.1842	0.149*
H17B	0.1887	0.0399	−0.3270	0.149*
H17C	0.2223	0.1080	−0.3117	0.149*
C18	0.26051(19)	−0.0439(2)	−0.2592(4)	0.0896(12)
H18A	0.2919	−0.0536	−0.3170	0.134*
H18B	0.2272	−0.0561	−0.3073	0.134*
H18C	0.2632	−0.0698	−0.1751	0.134*
C19	0.49358(10)	0.14208(11)	0.1106(3)	0.0466(5)
C20	0.50692(12)	0.13149(15)	−0.0266(3)	0.0608(7)
H20	0.4791	0.1223	−0.0904	0.073*
C21	0.56167(14)	0.13448(17)	−0.0704(4)	0.0760(9)
H21	0.5704	0.1279	−0.1633	0.091*
C22	0.60277(13)	0.14725(17)	0.0240(5)	0.0773(10)
H22	0.6394	0.1493	−0.0055	0.093*
C23	0.59065(13)	0.15701(17)	0.1609(4)	0.0724(9)
H23	0.6189	0.1652	0.2242	0.087*
C24	0.53650(12)	0.15470(14)	0.2048(3)	0.0600(7)
H24	0.5283	0.1616	0.2979	0.072*
C25	0.42184(12)	0.07785(13)	0.3068(3)	0.0520(6)
C26	0.45628(15)	0.02112(15)	0.3015(3)	0.0687(8)
H26	0.4837	0.0180	0.2343	0.082*
C27	0.44915(19)	−0.03175(18)	0.3994(4)	0.0910(12)
H27	0.4718	−0.0701	0.3962	0.109*
C28	0.4093(2)	−0.0268(2)	0.4984(5)	0.1041(15)

Table 2 (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
H28	0.4047	−0.0621	0.5619	0.125*
C29	0.3764(2)	0.0288(2)	0.5054(4)	0.1064(14)
H29	0.3499	0.0322	0.5750	0.128*
C30	0.38211(16)	0.08114(18)	0.4085(3)	0.0752(9)
H30	0.3587	0.1188	0.4128	0.090*
B1	0.1546(3)	0.2500	0.9675(7)	0.0918(19)
F1	0.1796(3)	0.2500	0.8544(5)	0.237(4)
F2	0.1900(3)	0.2500	1.0590(7)	0.359(8)
F3	0.1238(3)	0.2992(3)	0.9858(7)	0.283(3)

tetrahedral with two N—Cu—P bond angles of 107.85(3)° and 112.73(3)° and a 2,2'-bipyridine bite angle of 78.78(12)°. The P—Cu—P bond angle is 126.17(3)°. The Cu—N and Cu—P bond distances are similar to those reported for other copper(I) complexes [7]. Both intra and intermolecular non-classical hydrogen bonding interactions take place. The 2,2'-bipyridine ligand is engaged in CH_{phenyl}⋯N_{bipy} (C⋯N: 3.599(4) Å) interactions with two phosphine phenyl groups in addition to CH_{bipy}⋯F (C⋯F: 3.325(7) Å) interactions with the counterion BF₄[−]. The nitrogen atom of the dimethylamino group is essentially coplanar with the three carbon atoms, the deviation from the mean plane being 0.059(3) Å. The N3—C14 bond distance (1.375(3) Å) is significantly shorter than N3—C17 and N3—C18 bond distances (1.440(5) Å and 1.446(5) Å).

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