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Crystal structure of bis[(((4-fluorophenyl)amino)methyl)triphenylphosphonium] tetrachloridocobaltate(II), $C_{50}H_{44}Cl_4CoF_2N_2P_2$

Table 1: Data collection and handling.

Crystal:	Blue fragment
Size:	0.40 × 0.34 × 0.33 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.71 mm ⁻¹
Diffractometer, scan mode:	Bruker Kappa APEX-II DUO CCD, φ and ω
$\theta_{\max}$, completeness:	28.9°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	198347, 12366, 0.043
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 10091
$N(\text{param})_{\text{refined}}$:	556
Programs:	Bruker [1, 2], SHELX [3, 4]

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Abstract

$C_{50}H_{44}Cl_4CoF_2N_2P_2$, orthorhombic, *Pbca* (no. 61), $a = 18.4662(6)$ Å, $b = 15.2888(5)$ Å, $c = 33.2661(10)$ Å, $V = 9391.9(5)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0403$, $wR_{\text{ref}}(F^2) = 0.1005$, $T = 180.0(5)$ K.

CCDC no.: 1855274

The asymmetric unit of the title 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.

Source of material

An ethanol solution of $[CoCl_2(PPh_3)_2]$ (0.2 mmol) in ethanol (25 mL) and the Schiff base 2-[(4-fluorophenylimino)-methyl]-phenol (0.2 mmol) in 1:1 molar ratio was added and heated under reflux in a round bottom flask fitted with a double surface condenser for 6 h. The solution was then concentrated on the water bath to 3 mL and cooled. The product {bis[(((4-fluorophenyl)amino)methyl)triphenylphosphonium] tetrachloridocobaltate(II)} was precipitated by the addition of small quantity of petroleum ether (60–80 °C) and recrystallized from CH_2Cl_2 /petroleum ether and dried in vacuum (Yield-70–16%). Anal. calcd. for $C_{50}H_{44}CoN_2P_2F_2Cl_4$ (%): C, 61.68; H, 4.55; N, 2.87. Found (%): C, 61.63; H, 4.25; N, 2.75.

Experimental details

Hydrogen atoms were treated by a mixture of independent and constrained refinement. Coordinates for NH hydrogen atoms were refined, while those on C were placed in idealized positions. U_{iso} values for H were assigned as 1.2 time the U_{eq} values for the atoms to which they are bonded.

Comment

Schiff base ligands play a vital role in preparation of synthetic drugs and biological processes. These bioactive compounds have attracted their attention in the field of anti-cancer [5, 6] anti malarial [7, 8] and various clinical and pharmacological areas [9–13]. They gained attraction in the field of super capacitors, organic solar cells, electro chromic

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Co1	0.13917(2)	0.48030(2)	0.37476(2)	0.03734(7)
Cl1	0.04392(2)	0.38797(3)	0.35873(2)	0.03274(10)
Cl2	0.14222(3)	0.49633(3)	0.44253(2)	0.03928(11)
Cl3	0.24069(3)	0.41119(5)	0.35304(2)	0.05812(17)
Cl4	0.12414(6)	0.60710(5)	0.34281(3)	0.1031(4)
P1	0.19516(2)	0.20962(3)	0.26076(2)	0.03027(10)
F1	−0.01012(7)	−0.08440(9)	0.40520(4)	0.0528(3)
N1	0.10579(8)	0.19899(11)	0.32431(5)	0.0326(3)
H1N	0.0911(12)	0.2470(15)	0.3343(7)	0.039*
C1	0.18233(10)	0.20545(13)	0.31515(5)	0.0325(4)
H1C	0.2082	0.1542	0.3263	0.039*
H1D	0.2026	0.2589	0.3276	0.039*
C2	0.07739(9)	0.12505(12)	0.34398(5)	0.0291(4)
C3	0.10529(11)	0.04163(13)	0.33886(6)	0.0372(4)
H3	0.1450	0.0327	0.3212	0.045*
C4	0.07583(11)	−0.02901(14)	0.35935(6)	0.0394(4)
H4	0.0956	−0.0859	0.3562	0.047*
C5	0.01777(10)	−0.01538(14)	0.38425(6)	0.0370(4)
C6	−0.01245(10)	0.06585(14)	0.38938(6)	0.0343(4)
H6	−0.0534	0.0736	0.4063	0.041*
C7	0.01777(9)	0.13622(13)	0.36940(5)	0.0301(4)
H7	−0.0022	0.1929	0.3730	0.036*
C8	0.15004(9)	0.30263(12)	0.23955(5)	0.0311(4)
C9	0.13642(10)	0.37591(13)	0.26295(6)	0.0336(4)
H9	0.1476	0.3755	0.2908	0.040*
C10	0.10635(11)	0.44996(14)	0.24542(7)	0.0398(4)
H10	0.0972	0.5004	0.2613	0.048*
C11	0.08972(12)	0.45054(15)	0.20499(7)	0.0459(5)
H11	0.0682	0.5009	0.1933	0.055*
C12	0.10427(15)	0.37819(17)	0.18154(7)	0.0529(6)
H12	0.0934	0.3791	0.1536	0.063*
C13	0.13460(13)	0.30449(15)	0.19856(6)	0.0451(5)
H13	0.1450	0.2550	0.1823	0.054*
C14	0.28984(10)	0.21847(14)	0.24911(7)	0.0402(5)
C15	0.31398(15)	0.19241(18)	0.21142(9)	0.0667(8)
H15	0.2811	0.1679	0.1926	0.080*
C16	0.38613(19)	0.2024(2)	0.20160(13)	0.0866(12)
H16	0.4029	0.1849	0.1758	0.104*
C17	0.43360(15)	0.2371(2)	0.22871(12)	0.0893(13)
H17	0.4834	0.2423	0.2219	0.107*
C18	0.40992(13)	0.2646(3)	0.26557(11)	0.0919(13)
H18	0.4431	0.2897	0.2841	0.110*
C19	0.33721(12)	0.2557(2)	0.27605(8)	0.0661(8)
H19	0.3205	0.2752	0.3015	0.079*
C20	0.15970(11)	0.11195(13)	0.23911(6)	0.0352(4)
C21	0.08895(12)	0.10882(15)	0.22442(6)	0.0423(5)
H21	0.0595	0.1597	0.2251	0.051*
C22	0.06170(14)	0.03189(17)	0.20889(7)	0.0519(6)
H22	0.0136	0.0300	0.1987	0.062*
C23	0.10399(17)	−0.04192(18)	0.20806(8)	0.0620(7)
H23	0.0853	−0.0947	0.1971	0.074*
C24	0.17352(17)	−0.03969(17)	0.22303(9)	0.0653(7)
H24	0.2022	−0.0912	0.2226	0.078*
C25	0.20192(14)	0.03669(15)	0.23863(8)	0.0514(6)
H25	0.2499	0.0378	0.2489	0.062*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
P2	0.48848(3)	0.78152(3)	0.50573(2)	0.03103(10)
F2	0.83431(8)	0.94565(16)	0.41007(6)	0.0913(6)
N2	0.55148(9)	0.84922(12)	0.43969(5)	0.0367(4)
H2N	0.5273(13)	0.8537(16)	0.4192(7)	0.044*
C26	0.51224(10)	0.87635(12)	0.47507(6)	0.0340(4)
H26A	0.4676	0.9076	0.4670	0.041*
H26B	0.5424	0.9171	0.4910	0.041*
C27	0.62414(10)	0.87217(12)	0.43354(6)	0.0319(4)
C28	0.67038(11)	0.89506(14)	0.46470(6)	0.0373(4)
H28	0.6534	0.8939	0.4917	0.045*
C29	0.74114(12)	0.91956(16)	0.45662(7)	0.0483(5)
H29	0.7727	0.9361	0.4779	0.058*
C30	0.76493(11)	0.91963(19)	0.41791(8)	0.0550(6)
C31	0.72192(13)	0.89376(19)	0.38657(7)	0.0552(6)
H31	0.7403	0.8926	0.3599	0.066*
C32	0.65160(11)	0.86951(16)	0.39445(6)	0.0440(5)
H32	0.6213	0.8507	0.3730	0.053*
C33	0.43802(11)	0.81987(13)	0.54829(6)	0.0360(4)
C34	0.37080(12)	0.78393(15)	0.55741(7)	0.0451(5)
H34	0.3520	0.7372	0.5418	0.054*
C35	0.33147(14)	0.81685(18)	0.58949(8)	0.0549(6)
H35	0.2855	0.7925	0.5958	0.066*
C36	0.35848(14)	0.88467(17)	0.61227(7)	0.0542(6)
H36	0.3312	0.9067	0.6343	0.065*
C37	0.42480(15)	0.92055(16)	0.60320(7)	0.0537(6)
H37	0.4432	0.9674	0.6189	0.064*
C38	0.46480(13)	0.88881(15)	0.57136(7)	0.0466(5)
H38	0.5105	0.9139	0.5652	0.056*
C39	0.57041(10)	0.72839(13)	0.52012(7)	0.0418(5)
C40	0.61079(13)	0.68662(14)	0.49027(10)	0.0561(7)
H40	0.5934	0.6833	0.4634	0.067*
C41	0.67736(15)	0.64991(16)	0.50087(13)	0.0789(11)
H41	0.7063	0.6217	0.4811	0.095*
C42	0.70109(15)	0.65484(19)	0.54053(15)	0.0893(13)
H42	0.7459	0.6288	0.5478	0.107*
C43	0.66123(16)	0.6963(2)	0.56906(13)	0.0839(11)
H43	0.6787	0.6996	0.5959	0.101*
C44	0.59570(13)	0.73346(17)	0.55941(9)	0.0588(7)
H44	0.5679	0.7624	0.5794	0.071*
C45	0.43316(10)	0.70808(13)	0.47737(6)	0.0345(4)
C46	0.38260(11)	0.74060(15)	0.45014(7)	0.0415(5)
H46	0.3801	0.8015	0.4447	0.050*
C47	0.33581(12)	0.68283(18)	0.43100(7)	0.0515(6)
H47	0.3011	0.7044	0.4124	0.062*
C48	0.33943(13)	0.59433(18)	0.43887(8)	0.0560(7)
H48	0.3070	0.5553	0.4258	0.067*
C49	0.38998(13)	0.56233(16)	0.46562(8)	0.0527(6)
H49	0.3928	0.5012	0.4706	0.063*
C50	0.43664(12)	0.61866(14)	0.48529(7)	0.0426(5)
H50	0.4708	0.5966	0.5041	0.051*

materials, organic light-emitting diodes and nonlinear optic materials [14–19].

The asymmetric unit of the title structure contains, two phosphonium cations and one tetrachloridocobaltate(II)

dianion (see the figure). The bond lengths and angles within these moieties are in the expected ranges.

The four chlorido ligands (Cl1–Cl4) of the tetrachloridocobaltate(II) anion show Co–Cl distances ranging from 2.2282(7) Å to 2.3175(5) Å whereas the Co–Cl4 bond length with 2.2282(7) Å is the shortest of them.

This finding is in accord with the hydrogen bonding scheme of the title structure. The chlorido ligands Cl1 and Cl2 form classical $NH \cdots Cl$ hydrogen bonds. The chlorido ligand Cl4 does not form any hydrogen bond and additionally shows a large amplitude of the displacement ellipsoid perpendicular to the Co–Cl bond, furthermore artefactually reducing the derived bond length (see the figure).

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