Inorganic Chemistry
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Supporting Information

Experimental Procedure

2,6-bis(5-methylpyrazol-3-yl)pyridine (2.00 g, 8.36 mmol, prepared by reacting hydrazine hydrate with the product of the reaction of dimethylacetamide dimethyl acetal with 2,6-diacetylpyridine.[12] A full report of the preparation of this triheterocycle will appear subsequently.) was dissolved in diglyme (150 ml) and treated with potassium (0.654 g, 16.7 mmol). The reaction mixture was heated to 70° C to dissolve the potassium metal. 2-Bromopyridine (2.65 g (1.60 mL), 16.8 mmol) was added when the metal had dissolved. The reaction mixture was heated at 120 °C for 7 days. After cooling the mixture, the solvent was removed by rotary evaporation and the residue was washed with water. The solid was collected and dried. Purification was achieved by dissolving the solid in a minimum volume of dichloromethane, adding methanol (*ca.* 10 mL) and rotary evaporating the dichloromethane. The compound (1bmppp) was collected and washed with cold methanol (yield 0.81 g, 24.5%). MS (CI, CH_4): m/z values (abundance): 394 ($[M+H]^+$, 100%), 395 ($[M+2H]^+$, 23%). Analysis: C 70.2%, H 4.9%, N 24.9%; 1bmppp $C_{23}H_{19}N_7$ requires C 70.0%, H 5.1%, N 24.9%. Melting Point 196-197°C. ^{1}H NMR (200.132 MHz, $CDCl_3$): δ = 8.48 (ddd, 2H, H_6, $J_{4,6}$ = 1.0 Hz, $J_{5,6}$ = 4.9 Hz), 7.21 (ddt, 2H, H_5, $J_{3,5}$ = 1.2 Hz, $J_{4,5}$ = 7.4 Hz), 7.85 (ddt, 2H, H_4, $J_{3,4}$ = 8.1 Hz), 8.04 (d, 2H, H_3), 2.77 (s, 6H, CH_3 group), 7.02 (s, pyrazolyl proton), 8.04 (d, 2H, $H_{3'}$, $J_{3',4'}$ = 7.4 Hz), 7.79 (t, 1H, $H_{4'}$). ^{13}C NMR (50.323 MHz, $CDCl_3$): δ = 153.7 (2), 116.3 (3), 138.3 (4), 119.1 (5), 147.5 (6), 151.5 (pyrazole 3), 107.8 (pyrazole 4), 142.3 (pyrazole 5), 14.6 (methyl group), 152.5 (2'), 121.2 (3'), 136.9 (4').

1Bmppp (100 mg, 0.255 mmol) and tetrakis(acetonitrile)copper(I) hexafluorophosphate (142 mg, 0.382 mmol) were heated in boiling methanol (20 mL) On cooling the brown complex precipitated. The complex was collected and washed with cold methanol. Analysis: C 39.9%, H 3.3%, N 14.6%; $[Cu_3(C_{23}H_{19}N_7)_2(CH_3CN)_2](PF_6)_3$ ($C_{50}H_{44}Cu_3F_{18}N_{16}P_3$) requires C 40.2%, H 3.0%, N 15.0%. MS(FAB, 3-nitrobenzylalcohol): m/z values (abundance): 1265

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$[Cu_3(1bmppp)_2(PF_6)_2^+]$ (3%), 1139 $[Cu_2(1bmppp)_2(CH_3CN)_2(PF_6)^+]$ (2%), 1057 $[Cu_2(1bmppp)_2(PF_6)^+]$ (6%), 994 $[Cu_2(1bmppp)_2(CH_3CN)_2^+]$ (2.5 %), 912 $[Cu_2(1bmppp)_2^+]$ (3%), 456 $[Cu(1bmppp)^+]$ (100%). The assignment of the ions was confirmed by inspection of isotope patterns for the proposed formulations, the masses quoted are based on ^1H, ^{12}C, ^{63}Cu, ^{14}N, ^{31}P and ^{19}F. Electrospray ionisation mass spectroscopy (ES-MS) exhibits similar peaks m/z 456 $[Cu(1bmppp)^+]$, 849 $[Cu(1bmppp)_2^+]$ and 1059 $[Cu_2(1bmppp)_2(PF_6)^+]$. ^1H NMR (300.132 MHz, $CDCl_3$): $\underline{\delta}$ = 8.21 (d, 2H, H_6, $\underline{J_{5,6}}$ = 4.1 Hz), 7.31 (t, 2H, H_5, $\underline{J_{4,5}}$ = 7.1 Hz), 7.7 (dt, 2H, H_4, $\underline{J_{3,4}}$ = 8.2 Hz), 7.43 (d, 2H, H_3), 2.53 (s, 6H, CH_3 group), 6.68 (s, pyrazolyl proton), 7.64 (d, 2H, $H_{3'}$, $\underline{J_{3',4'}}$ = 7.4 Hz), 8.00 (t, 1H, $H_{4'}$). UV-Vis solid state reflectance spectrum: $\underline{\lambda_{max}}$ 445 nm. Crystals were grown for the structure determination by vapour diffusion of diethyl ether into an acetonitrile solution of the complex.

Crystal Structure Determination

Crystal data $[Cu_3(C_{23}H_{19}N_7)_2(CH_3CN)_2](PF_6)_3$, M 1494.5, monoclinic, space group C2/c, a 15.330(7), b 20.847(5), c 19.100(9) Å, β 101.95(2)°, V 5972(4) Å^3, D_c 1.66 g cm^{-3}, Z 4, μ_{Mo} 12.45 cm^{-1}. Crystal size 0.09 by 0.09 by 0.26 mm, $2\theta_{max}$ 50°, min. and max. transmission factors: 0.74 and 0.89. The number of reflections was 2810 considered observed ($I > 3\sigma(I)$) out of 5232 unique data, with R_{merge} 0.029 for 125 pairs of equivalent 0kl reflections . Final residuals R, R_w were 0.063, 0.082 for the observed data.

Structure Determination Reflection data were measured with an Enraf-Nonius CAD-4 diffractometer in θ/2θ scan mode using graphite monochromatized molybdenum radiation (λ 0.7107Å). Data were corrected for absorption using the method of de Meulenaer and Tompa.[1] The structure was determined by direct phasing and Fourier methods. Hydrogen atoms were included in calculated positions and were assigned thermal parameters equal to those of the atom to which they were bonded. The PF_6^- groups were poorly defined, with the anion at the general position being disordered. The anions were modelled as three identical octahedra with a common refineable P - F distance (final value 1.550(3) Å). One octahedron was used to describe the group on the 2-fold axis, and two independent overlapping octahedra described the disorder of the other. The final occupancies of the disordered anions were 0.69(2) and 0.31(2) for orientations B and B', respectively. The group thermal motions were described by rigid body 15 parameter TLX models. The remaining non-hydrogen atoms were refined with individual positional and anisotropic thermal parameters . Reflection weights used were $1/\sigma^2(F_o)$, with $\sigma(F_o)$ being derived from $\sigma(I_o) = [\sigma^2(I_o) + (0.04I_o)^2]^{1/2}$. The residue is defined as $R = \Sigma\Delta/\Sigma|F_o|$ and the weighted residual is defined as $R_w=(\Sigma w\Delta^2/\Sigma wF_o^2)^{1/2}$. Atomic scattering factors and anomalous dispersion parameters were from International Tables for X-ray Crystallography.[2] Structure solution was by MULTAN80[3] and refinement used RAELS94.[4] ORTEP-II[5] running on a Macintosh IIcx was used for the structural diagram, and a DEC Alpha-AXP workstation was used for calculations.

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Further details of the crystal structure investigation are available on request from the Director of the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK on quoting the full journal citation.

References

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(3) Main, P. *MULTAN80*, University of York, York, England, **1980**.

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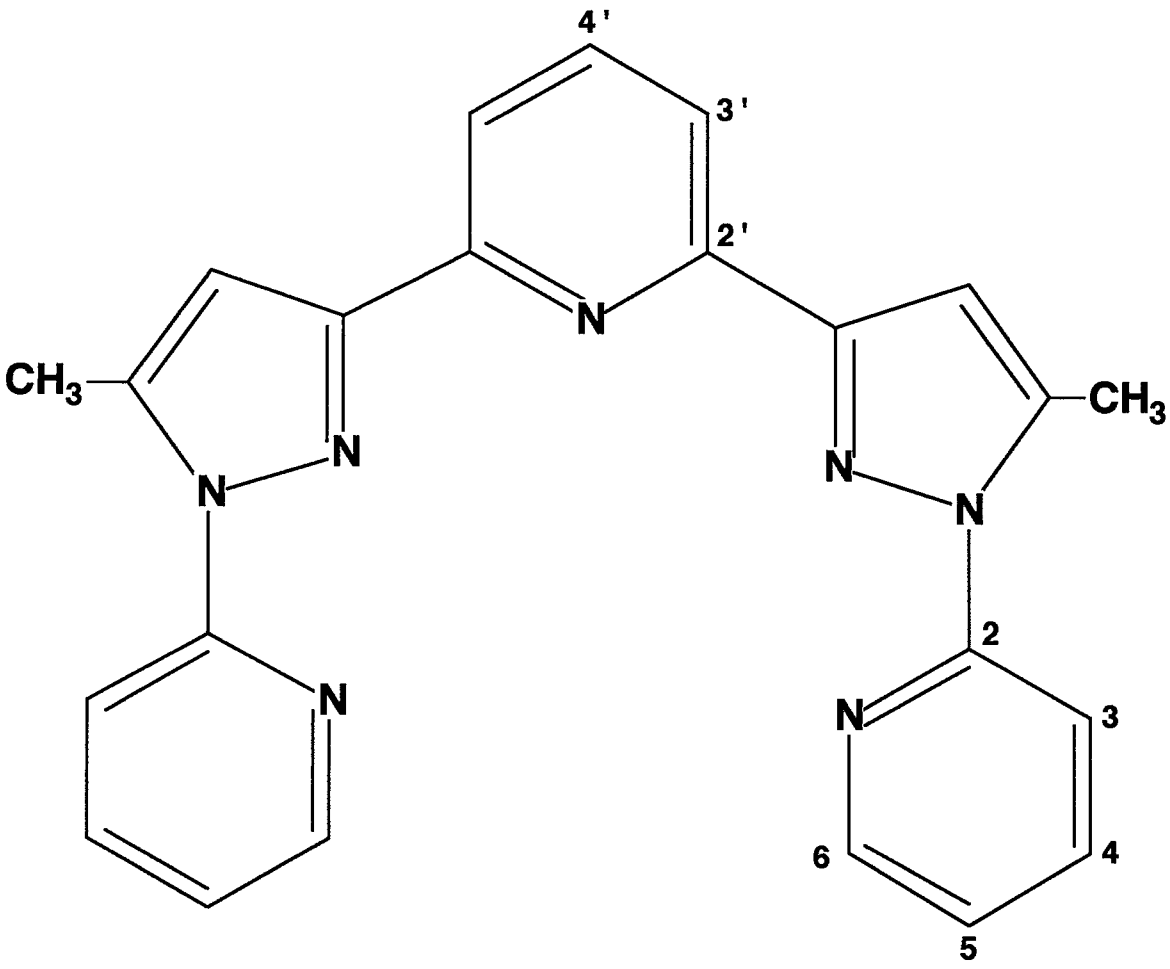
(5) Johnson, C. K. *ORTEP-II*, Oak Ridge National Laboratory, Tennessee, USA, **1976**.

P1092-MS

Scheme



Scheme 1. 1bmppp. The numbering scheme is referred to in the ^{1}H and ^{13}C nmr interpretation.

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Figure

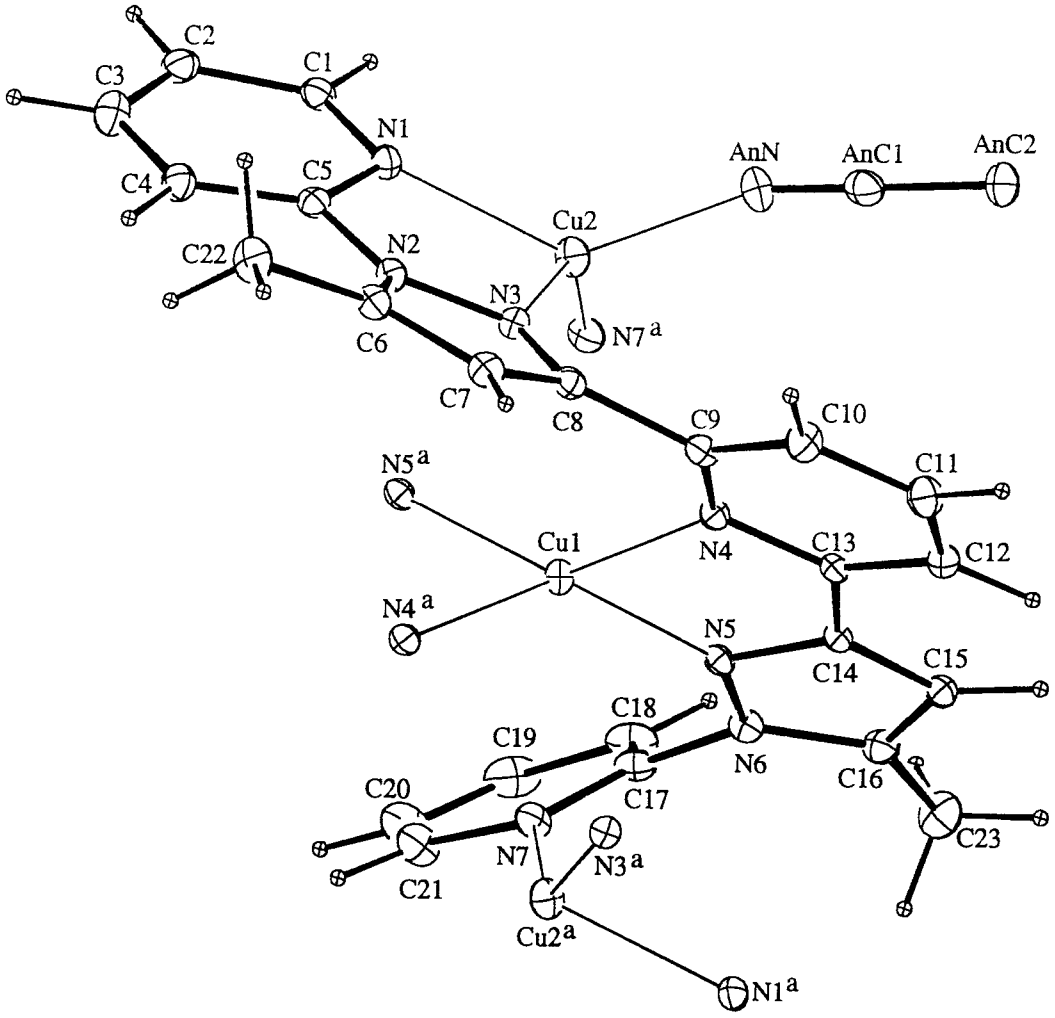

Figure 1. Full labelling scheme for the complex trinuclear cation.

P-1092-MM

Table 1. Non-hydrogen atomic parameters for $[Cu_3(lbmppp)_2(CH_3CN)_2][PF_6]_3$. Esd i parentheses.

	x	y	z	$(U_{11}+U_{22}+U_{33})/3$
Cu1	0.50000	0.17412(7)	0.25000	0.046(1)
Cu2	0.40852(8)	0.16225(5)	0.08304(6)	0.056(1)
N1	0.2701(5)	0.1737(4)	0.0620(4)	0.048(2)
N2	0.3083(5)	0.2704(3)	0.1191(4)	0.040(2)
N3	0.3948(5)	0.2507(3)	0.1258(4)	0.040(2)
N4	0.5713(5)	0.2351(3)	0.1947(3)	0.039(2)
N5	0.6191(5)	0.1319(3)	0.2691(3)	0.040(2)
N6	0.6554(5)	0.0761(3)	0.2989(4)	0.047(2)
N7	0.5593(5)	0.0710(4)	0.3790(4)	0.054(2)
C1	0.2098(7)	0.1283(5)	0.0369(5)	0.051(2)
C2	0.1204(7)	0.1316(5)	0.0428(5)	0.062(3)
C3	0.0944(7)	0.1839(5)	0.0768(6)	0.070(3)
C4	0.1549(6)	0.2312(5)	0.1026(5)	0.057(3)
C5	0.2406(6)	0.2255(4)	0.0930(4)	0.044(2)
C6	0.3065(6)	0.3350(4)	0.1359(5)	0.050(2)
C7	0.3931(7)	0.3545(4)	0.1541(5)	0.052(2)
C8	0.4461(6)	0.3005(5)	0.1484(4)	0.046(2)
C9	0.5440(6)	0.2914(4)	0.1636(4)	0.046(2)
C10	0.6019(7)	0.3350(4)	0.1439(5)	0.059(3)
C11	0.6902(7)	0.3198(5)	0.1546(5)	0.064(3)
C12	0.7207(6)	0.2613(5)	0.1851(5)	0.054(2)
C13	0.6586(6)	0.2210(4)	0.2047(4)	0.039(2)
C14	0.6824(6)	0.1587(4)	0.2403(4)	0.040(2)
C15	0.7598(6)	0.1204(5)	0.2527(5)	0.052(2)
C16	0.7412(7)	0.0677(5)	0.2898(5)	0.055(3)
C17	0.6022(7)	0.0392(4)	0.3354(5)	0.052(2)
C18	0.5926(8)	-0.0269(5)	0.3237(5)	0.071(3)
C19	0.5339(10)	-0.0585(5)	0.3599(7)	0.089(4)
C20	0.4868(9)	-0.0254(6)	0.4008(7)	0.090(4)
C21	0.4994(7)	0.0383(5)	0.4084(6)	0.069(3)
C22	0.2228(7)	0.3732(5)	0.1318(6)	0.070(3)
C23	0.7969(7)	0.0109(5)	0.3162(6)	0.077(3)
AnN	0.4961(6)	0.1779(4)	0.0207(5)	0.068(2)
AnC1	0.5586(8)	0.1964(5)	0.0043(5)	0.064(3)
AnC2	0.6391(7)	0.2241(6)	-0.0173(6)	0.087(4)
PA	0.5000	0.2289(1)	0.7500	0.059(1)
F1A	0.5709(1)	0.1764(2)	0.7478(2)	0.100(2)
F2A	0.4748(4)	0.2289(1)	0.6671(2)	0.130(2)
F3A	0.4291(1)	0.2815(2)	0.7522(2)	0.109(2)
F4A	0.5709(1)	0.2815(2)	0.7478(2)	0.109(2)
F5A	0.4291(1)	0.1764(2)	0.7522(2)	0.100(2)
F6A	0.5252(4)	0.2289(1)	0.8329(2)	0.130(2)
PB	0.2040(5)	0.0640(2)	0.4541(3)	0.115(5)
F1B	0.1378(7)	0.0230(5)	0.4865(6)	0.227(7)
F2B	0.2303(9)	0.1015(5)	0.5254(4)	0.231(7)
F3B	0.2702(8)	0.1049(5)	0.4217(5)	0.181(6)
F4B	0.1777(9)	0.0265(5)	0.3828(4)	0.220(7)
F5B	0.1292(7)	0.1134(5)	0.4268(8)	0.262(8)
F6B	0.2789(7)	0.0146(4)	0.4814(7)	0.203(6)
PB'	0.1741(13)	0.0679(6)	0.4445(9)	0.136(5)
F1B'	0.2374(20)	0.0667(13)	0.5191(9)	0.189(6)
F2B'	0.0983(19)	0.0948(15)	0.4785(21)	0.360(13)
F3B'	0.1436(20)	-0.0014(9)	0.4565(17)	0.200(7)
F4B'	0.1108(20)	0.0690(15)	0.3698(14)	0.309(11)
F5B'	0.2499(19)	0.0410(12)	0.4104(13)	0.186(6)
F6B'	0.2046(21)	0.1371(7)	0.4325(16)	0.199(6)

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Table 2. Hydrogen atom positional parameters for $[Cu_3(lbmppp)_2(CH_3CN)_2][PF_6]_3$.

Thermal parameters equal to those of bonded atom.

	x	y	z
HC1	0.2298	0.0901	0.0128
HC2	0.0771	0.0970	0.0229
HC3	0.0313	0.1876	0.0828
HC4	0.1366	0.2693	0.1280
HC7	0.4148	0.3987	0.1687
HC10	0.5796	0.3771	0.1221
HC11	0.7332	0.3509	0.1405
HC12	0.7850	0.2490	0.1925
HC15	0.8171	0.1298	0.2374
HC18	0.6256	-0.0503	0.2915
HC19	0.5267	-0.1061	0.3553
HC20	0.4435	-0.0480	0.4249
HC21	0.4628	0.0627	0.4371
H1C22	0.2385	0.4185	0.1464
H2C22	0.1872	0.3725	0.0816
H3C22	0.1869	0.3540	0.1647
H1C23	0.8566	0.0154	0.3034
H2C23	0.8046	0.0079	0.3694
H3C23	0.7670	-0.0288	0.2937

Table 3. Bond lengths (Å) for $[Cu_3(lbmppp)_2(CH_3CN)_2][PF_6]_3$. Esd in parentheses.

Cu1-Cu2	3.216(1)	C2-C3	1.370(14)
Cu1-N4	2.099(7)	C3-C4	1.375(13)
Cu1-N5	1.992(7)	C4-C5	1.368(12)
Cu2-N1	2.090(7)	C6-C7	1.363(12)
Cu2-N3	2.045(7)	C6-C22	1.498(12)
Cu2-AnN	1.996(9)	C7-C8	1.405(12)
Cu2-N7[a]	2.060(7)	C8-C9	1.481(12)
N1-C1	1.340(11)	C9-C10	1.376(12)
N1-C5	1.353(10)	C10-C11	1.364(13)
N2-N3	1.368(8)	C11-C12	1.390(13)
N2-C5	1.411(10)	C12-C13	1.379(11)
N2-C6	1.386(11)	C13-C14	1.475(11)
N3-C8	1.319(10)	C14-C15	1.409(12)
N4-C9	1.342(10)	C15-C16	1.369(13)
N4-C13	1.346(9)	C16-C23	1.486(13)
N5-N6	1.361(9)	C17-C18	1.399(12)
N5-C14	1.334(10)	C18-C19	1.407(16)
N6-C16	1.373(11)	C19-C20	1.358(17)
N6-C17	1.407(11)	C20-C21	1.346(15)
N7-C17	1.338(11)	AnN-AnC1	1.136(12)
N7-C21	1.356(11)	AnC1-AnC2	1.497(15)
C1-C2	1.400(13)	P-F	1.550(3)

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Table 4. Bond angles (°) for $[Cu_3(lbmppp)_2(CH_3CN)_2][PF_6]_3$. Esd in parentheses.

N4-Cu1-N5	78.9(3)	N2-C5-C4	123.5(8)
N4-Cu1-N5[a]	136.8(3)	N2-C6-C7	106.4(8)
N4-Cu1-N4[a]	105.4(4)	N2-C6-C22	124.2(8)
N5-Cu1-N5[a]	127.5(4)	C7-C6-C22	129.4(9)
N1-Cu2-N3	77.8(3)	C6-C7-C8	106.8(8)
N1-Cu2-AnN	130.4(3)	N3-C8-C7	109.9(8)
N1-Cu2-N7[a]	109.5(3)	N3-C8-C9	118.3(8)
N3-Cu2-AnN	103.2(3)	C7-C8-C9	131.7(9)
N3-Cu2-N7[a]	136.8(3)	N4-C9-C8	114.1(8)
AnN-Cu2-N7[a]	102.7(3)	N4-C9-C10	122.6(9)
Cu2-N1-C1	125.8(6)	C8-C9-C10	123.2(8)
Cu2-N1-C5	115.2(6)	C9-C10-C11	118.8(9)
C1-N1-C5	116.8(8)	C10-C11-C12	120.3(9)
N3-N2-C5	117.5(6)	C11-C12-C13	117.2(8)
N3-N2-C6	109.7(7)	N4-C13-C12	123.4(8)
C5-N2-C6	132.7(7)	N4-C13-C14	113.8(7)
Cu2-N3-N2	114.3(5)	C12-C13-C14	122.9(8)
Cu2-N3-C8	137.4(6)	N5-C14-C13	115.3(7)
N2-N3-C8	107.1(7)	N5-C14-C15	110.6(8)
Cu1-N4-C9	127.3(6)	C13-C14-C15	134.1(8)
Cu1-N4-C13	113.7(5)	C14-C15-C16	106.4(8)
C9-N4-C13	117.7(7)	N6-C16-C15	105.8(8)
Cu1-N5-N6	137.2(6)	N6-C16-C23	123.9(9)
Cu1-N5-C14	117.1(5)	C15-C16-C23	130.4(10)
N6-N5-C14	105.2(7)	N6-C17-N7	116.6(8)
N5-N6-C16	112.0(7)	N6-C17-C18	120.8(10)
N5-N6-C17	116.5(7)	N7-C17-C18	122.6(10)
C16-N6-C17	131.4(8)	C17-C18-C19	116.1(11)
C17-N7-C21	118.1(8)	C18-C19-C20	121.0(10)
N1-C1-C2	123.5(9)	C19-C20-C21	118.8(11)
C1-C2-C3	117.5(9)	N7-C21-C20	123.1(11)
C2-C3-C4	120.0(9)	Cu2-AnN-AnC1	158.5(9)
C3-C4-C5	119.0(9)	AnN-AnC1-AnC2	177.1(12)
N1-C5-N2	113.3(7)	F-P-F	90.0
N1-C5-C4	123.1(9)		

Table 5. Torsional angles (°) for $[Cu_3(1bmppp)_2(CH_3CN)_2][PF_6]_3$. Esd in parenthe

N1-Cu2-Cu2[a]-N7	92.1(3)	N4-C13-C14-N5	-12.3(10)
N1-C5-N2-N3	-15.1(10)	N5-N6-C17-N7	-44.3(11)
N3-C8-C9-N4	-38.7(11)		

[a] indicates the symmetry transformation 1-x,y,1/2-z

$Cu_3(1bmppp)_2(CH_3CN)_2][PF_6]_3$

tomic parameters and standard deviations.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
u1	0.50000	0.17412(7)	0.25000	0.038(1)	0.047(1)	0.054(1)	0.000	0.004(1)	0.000
u2	0.40852(8)	0.16225(5)	0.08304(6)	0.055(1)	0.043(1)	0.068(1)	0.007(1)	0.007(1)	-0.001(1)
1	0.2701(5)	0.1737(4)	0.0620(4)	0.042(4)	0.053(5)	0.048(4)	0.005(4)	0.004(4)	0.000(4)
2	0.3083(5)	0.2704(3)	0.1191(4)	0.041(4)	0.033(4)	0.046(4)	0.007(4)	0.005(3)	0.003(3)
3	0.3948(5)	0.2507(3)	0.1258(4)	0.041(4)	0.034(4)	0.046(4)	0.001(4)	-0.001(3)	0.000(3)
4	0.5713(5)	0.2351(3)	0.1947(3)	0.042(4)	0.037(4)	0.040(4)	0.000(3)	0.003(3)	0.001(3)
5	0.6191(5)	0.1319(3)	0.2691(3)	0.045(4)	0.036(4)	0.039(4)	0.004(4)	0.007(4)	-0.003(3)
6	0.6554(5)	0.0761(3)	0.2989(4)	0.055(5)	0.039(4)	0.047(5)	0.004(4)	0.001(4)	0.002(4)
7	0.5593(5)	0.0710(4)	0.3790(4)	0.062(5)	0.048(5)	0.051(5)	-0.013(4)	0.005(4)	-0.001(4)
1	0.2098(7)	0.1283(5)	0.0369(5)	0.058(7)	0.053(6)	0.042(6)	-0.004(5)	0.005(5)	-0.005(5)
2	0.1204(7)	0.1316(5)	0.0428(5)	0.060(7)	0.075(8)	0.052(6)	-0.018(6)	-0.009(5)	0.004(6)
3	0.0944(7)	0.1839(5)	0.0768(6)	0.055(7)	0.063(7)	0.090(8)	0.002(6)	0.001(6)	0.009(6)
4	0.1549(6)	0.2312(5)	0.1026(5)	0.051(6)	0.057(6)	0.063(7)	0.007(6)	0.001(5)	0.003(5)
5	0.2406(6)	0.2255(4)	0.0930(4)	0.048(6)	0.043(5)	0.040(5)	0.008(5)	-0.001(4)	0.006(4)
6	0.3065(6)	0.3350(4)	0.1359(5)	0.054(6)	0.043(6)	0.052(6)	0.010(5)	0.006(5)	0.006(5)
7	0.3931(7)	0.3545(4)	0.1541(5)	0.058(6)	0.044(6)	0.054(6)	0.007(5)	0.002(5)	0.007(5)
8	0.4461(6)	0.3005(5)	0.1484(4)	0.047(6)	0.049(6)	0.043(6)	-0.002(5)	0.004(5)	0.006(4)
9	0.5440(6)	0.2914(4)	0.1636(4)	0.054(6)	0.046(6)	0.039(5)	-0.004(5)	0.004(4)	-0.001(4)
10	0.6019(7)	0.3350(4)	0.1439(5)	0.059(6)	0.047(6)	0.070(7)	-0.013(6)	0.001(5)	0.010(5)
11	0.6902(7)	0.3198(5)	0.1546(5)	0.060(7)	0.061(7)	0.072(7)	-0.021(6)	0.008(6)	0.010(6)
12	0.7207(6)	0.2613(5)	0.1851(5)	0.044(6)	0.068(7)	0.051(6)	-0.002(5)	0.001(5)	0.007(5)
13	0.6586(6)	0.2210(4)	0.2047(4)	0.039(5)	0.046(5)	0.033(5)	-0.001(4)	0.007(4)	-0.001(4)
14	0.6824(6)	0.1587(4)	0.2403(4)	0.038(5)	0.048(5)	0.034(5)	0.003(5)	0.003(4)	-0.006(4)
15	0.7598(6)	0.1204(5)	0.2527(5)	0.043(6)	0.071(7)	0.043(5)	0.007(5)	0.002(5)	-0.015(5)
16	0.7412(7)	0.0677(5)	0.2898(5)	0.061(7)	0.054(6)	0.050(6)	0.014(5)	-0.002(5)	0.002(5)
17	0.6022(7)	0.0392(4)	0.3354(5)	0.072(7)	0.039(6)	0.044(6)	0.004(5)	-0.009(5)	-0.004(4)
18	0.5926(8)	-0.0269(5)	0.3237(5)	0.113(10)	0.041(6)	0.061(7)	0.008(6)	-0.013(6)	-0.013(5)
19	0.5339(10)	-0.0585(5)	0.3599(7)	0.135(12)	0.049(7)	0.082(8)	-0.037(8)	-0.025(8)	0.015(7)
20	0.4868(9)	-0.0254(6)	0.4008(7)	0.124(12)	0.064(8)	0.083(9)	-0.039(8)	0.020(8)	-0.006(7)
21	0.4994(7)	0.0383(5)	0.4084(6)	0.084(8)	0.055(7)	0.070(7)	-0.032(6)	0.012(6)	-0.008(5)
22	0.2228(7)	0.3732(5)	0.1318(6)	0.068(7)	0.051(6)	0.092(8)	0.027(6)	0.010(6)	-0.002(6)
23	0.7969(7)	0.0109(5)	0.3162(6)	0.077(8)	0.058(7)	0.096(9)	0.025(6)	-0.004(7)	0.002(6)
nN	0.4961(6)	0.1779(4)	0.0207(5)	0.056(5)	0.069(6)	0.079(6)	0.003(5)	0.021(5)	0.001(5)
nC1	0.5586(8)	0.1964(5)	0.0043(5)	0.072(8)	0.067(7)	0.053(7)	0.021(7)	0.001(6)	-0.007(5)
nC2	0.6391(7)	0.2241(6)	-0.0173(6)	0.052(7)	0.126(11)	0.082(8)	-0.028(7)	0.008(6)	0.006(7)

A	0.5000	0.2289(1)	0.7500	0.045(2)	0.063(2)	0.068(3)	0.000	0.001(2)	0.000
1A	0.5709(1)	0.1764(2)	0.7478(2)	0.056(2)	0.078(2)	0.166(4)	0.013(2)	-0.001(2)	-0.007(2)
2A	0.4748(4)	0.2289(1)	0.6671(2)	0.182(7)	0.141(6)	0.068(3)	-0.001(1)	-0.004(2)	0.007(2)
3A	0.4291(1)	0.2815(2)	0.7522(2)	0.063(2)	0.078(2)	0.185(4)	0.017(2)	-0.004(3)	-0.009(3)
4A	0.5709(1)	0.2815(2)	0.7478(2)	0.063(2)	0.078(2)	0.185(4)	-0.017(2)	-0.004(3)	0.009(3)
5A	0.4291(1)	0.1764(2)	0.7522(2)	0.056(2)	0.078(2)	0.166(4)	-0.013(2)	-0.001(2)	0.007(2)
6A	0.5252(4)	0.2289(1)	0.8329(2)	0.182(7)	0.141(6)	0.068(3)	0.001(1)	-0.004(2)	-0.007(2)
B	0.2040(5)	0.0640(2)	0.4541(3)	0.210(8)	0.054(5)	0.082(7)	0.001(3)	0.040(7)	0.000(4)
1B	0.1378(7)	0.0230(5)	0.4865(6)	0.274(11)	0.176(12)	0.230(12)	-0.065(7)	0.095(8)	0.020(9)
2B	0.2303(9)	0.1015(5)	0.5254(4)	0.427(17)	0.149(8)	0.117(8)	-0.040(8)	0.083(8)	-0.062(5)
3B	0.2702(8)	0.1049(5)	0.4217(5)	0.276(8)	0.122(8)	0.146(9)	-0.051(6)	0.065(9)	0.023(5)
4B	0.1777(9)	0.0265(5)	0.3828(4)	0.423(17)	0.135(8)	0.101(8)	-0.058(8)	0.016(8)	-0.032(6)
5B	0.1292(7)	0.1134(5)	0.4268(8)	0.279(11)	0.115(10)	0.392(17)	0.038(8)	-0.057(11)	0.035(9)
6B	0.2789(7)	0.0146(4)	0.4814(7)	0.277(8)	0.081(6)	0.252(14)	0.017(6)	-0.033(9)	0.031(6)
B'	0.1741(13)	0.0679(6)	0.4445(9)	0.213(9)	0.068(5)	0.125(7)	0.002(3)	0.028(7)	0.005(4)
1B'	0.2374(20)	0.0667(13)	0.5191(9)	0.363(12)	0.128(7)	0.076(9)	-0.049(6)	0.041(6)	-0.004(3)
2B'	0.0983(19)	0.0948(15)	0.4785(21)	0.251(12)	0.250(20)	0.580(31)	0.055(9)	0.140(11)	-0.054(18)
3B'	0.1436(20)	-0.0014(9)	0.4565(17)	0.286(11)	0.111(7)	0.204(11)	-0.066(8)	0.012(10)	0.029(9)
4B'	0.1108(20)	0.0690(15)	0.3698(14)	0.464(20)	0.193(21)	0.270(13)	-0.086(12)	-0.182(15)	0.084(10)
5B'	0.2499(19)	0.0410(12)	0.4104(13)	0.289(8)	0.119(6)	0.150(10)	-0.002(6)	0.105(9)	-0.041(6)
6B'	0.2046(21)	0.1371(7)	0.4325(16)	0.322(13)	0.060(6)	0.216(10)	-0.005(4)	-0.021(12)	0.031(4)

ydrogen atoms. Thermal parameters assigned equal to those of atom to which bonded.

	x	y	z		x	y	z
C1	0.2298	0.0901	0.0128	HC19	0.5267	-0.1061	0.3553
C2	0.0771	0.0970	0.0229	HC20	0.4435	-0.0480	0.4249
C3	0.0313	0.1876	0.0828	HC21	0.4628	0.0627	0.4371
C4	0.1366	0.2693	0.1280	H1C22	0.2385	0.4185	0.1464
C7	0.4148	0.3987	0.1687	H2C22	0.1872	0.3725	0.0816
C10	0.5796	0.3771	0.1221	H3C22	0.1869	0.3540	0.1647
C11	0.7332	0.3509	0.1405	H1C23	0.8566	0.0154	0.3034
C12	0.7850	0.2490	0.1925	H2C23	0.8046	0.0079	0.3694
C15	0.8171	0.1298	0.2374	H3C23	0.7670	-0.0288	0.2937
C18	0.6256	-0.0503	0.2915				