Influence of anions on the dimensionality of extended networks based on Cu^{I} cations and 1,4,5,8,9,12-hexaazatriphenylene (HAT) ligands

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Supplementary materials

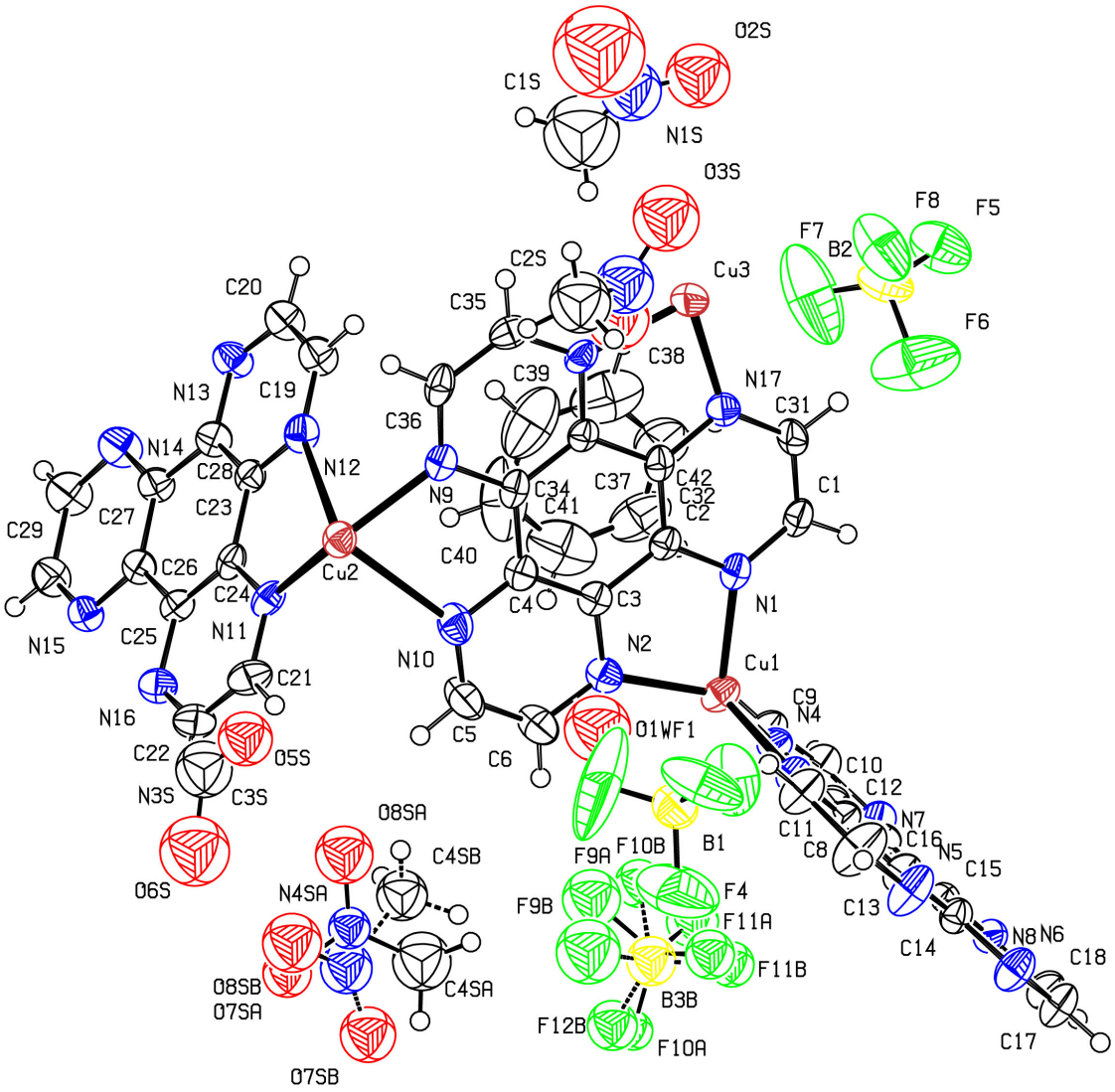

Fig. 1A. Thermal ellipsoid plot of the asymmetric unit in the crystal structure of **1** (50% probability ellipsoids).

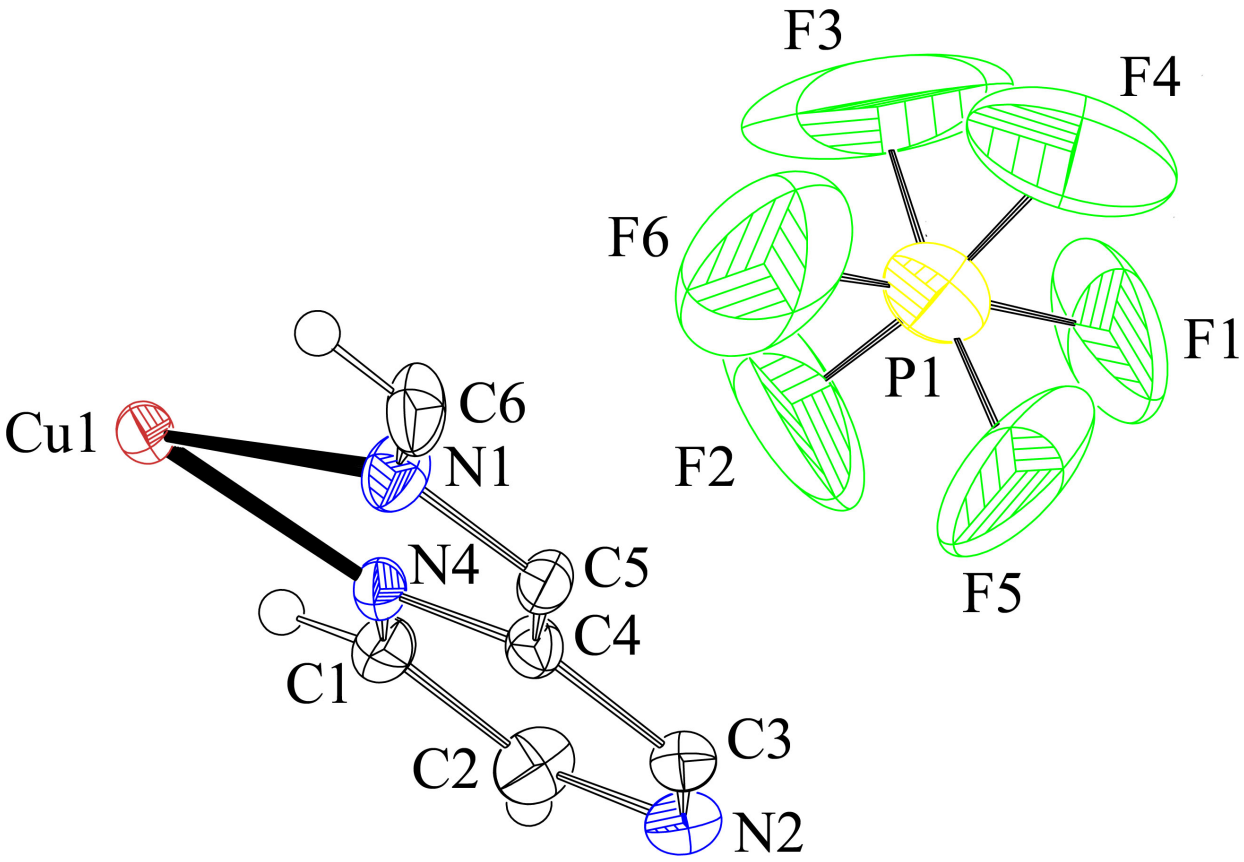

Fig. 2A. Thermal ellipsoid plot of the asymmetric unit in the crystal structure of **2** (50% probability ellipsoids).

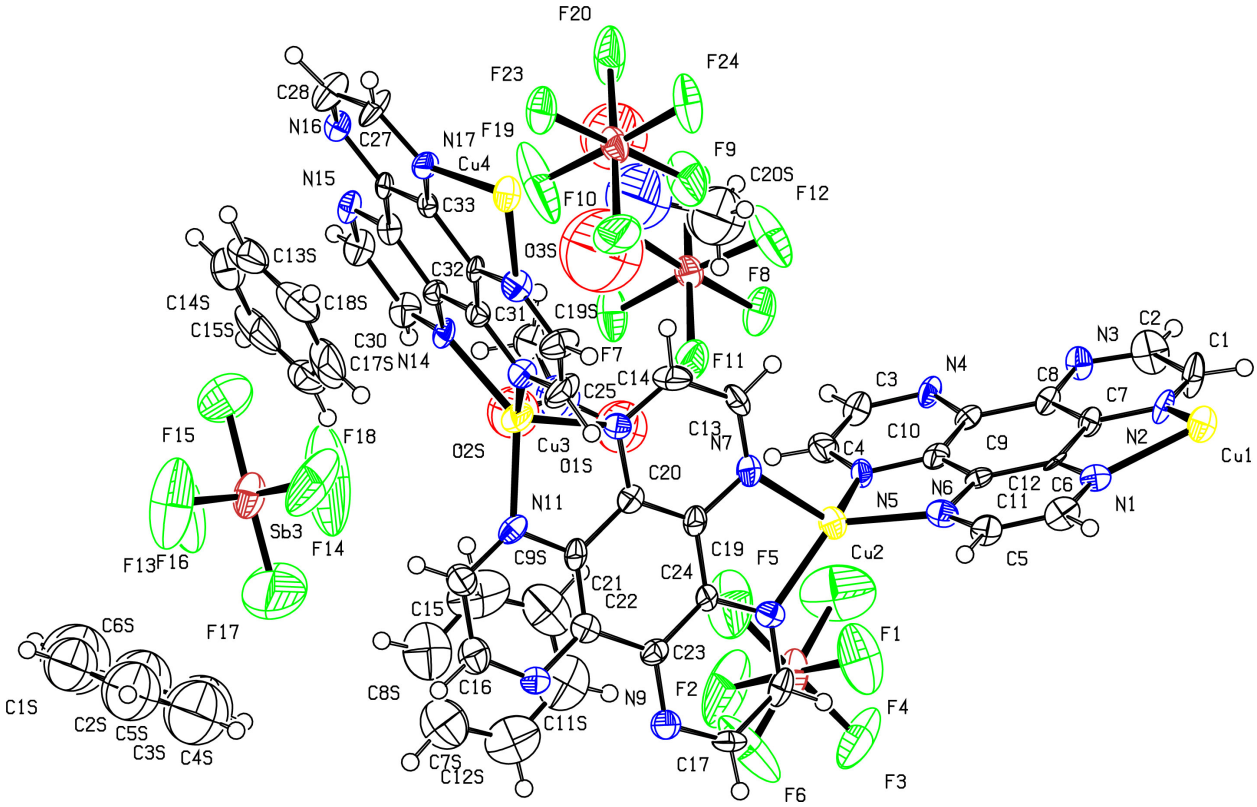

Fig. 3A. Thermal ellipsoid plot of the asymmetric unit in the crystal structure of **3** (50% probability ellipsoids).

Table 1A. Positional and thermal parameters for **1**.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	s.o.f.	U_{eq}
Cu(1)	0.33539(4)	0.64558(5)	0.14048(3)	1	0.0343(2)
Cu(2)	0.28384(5)	1.13268(5)	0.07970(3)	1	0.0322(2)
Cu(3)	0.17122(5)	1.16013(6)	-0.19972(3)	1	0.0389(2)
F(1)	0.3696(4)	0.9790(4)	0.2515(2)	1	0.0930(18)
F(2)	0.2764(4)	0.8685(5)	0.2135(2)	1	0.101(2)
F(3)	0.3575(8)	0.8375(5)	0.2938(4)	1	0.205(5)
F(4)	0.2658(5)	0.9488(6)	0.2872(3)	1	0.137(3)
F(5)	0.0181(3)	0.2157(4)	0.1796(2)	1	0.0769(15)
F(6)	-0.1010(4)	0.2055(5)	0.1997(4)	1	0.134(3)
F(7)	-0.0049(6)	0.1122(6)	0.2434(3)	1	0.158(4)
F(8)	-0.0628(4)	0.0812(4)	0.1562(2)	1	0.0944(19)
F(9A)	0.5712(7)	0.3533(8)	-0.0109(4)	0.61(1)	0.091(3)
F(10A)	0.5013(6)	0.2325(7)	0.0233(4)	0.61(1)	0.042(3)
F(11A)	0.6020(5)	0.1965(6)	-0.0149(3)	0.61(1)	0.073(3)
F(12A)	0.4773(6)	0.2567(8)	-0.0671(4)	0.61(1)	0.065(3)
F(9B)	0.4864(11)	0.3769(13)	-0.0208(7)	0.39(1)	0.111(7)
F(10B)	0.5957(8)	0.2981(10)	-0.0243(5)	0.39(1)	0.062(4)
F(11B)	0.4804(8)	0.2210(12)	-0.0665(6)	0.39(1)	0.056(4)
F(12B)	0.5065(12)	0.2547(14)	0.0301(8)	0.39(1)	0.067(6)
O(1S)	0.1757(14)	-0.0248(18)	0.4345(9)	0.72(1)	0.227(9)
O(2S)	0.1532(7)	0.1241(9)	0.4413(5)	0.72(1)	0.110(4)
O(3S)	0.3298(9)	0.0829(10)	0.4323(6)	0.64(1)	0.117(5)
O(4S)	0.3418(8)	0.1301(9)	0.3556(5)	0.64(1)	0.102(4)
O(5S)	0.4413(8)	0.4985(9)	0.4353(6)	0.5	0.079(4)
O(6S)	0.4028(11)	0.5318(14)	0.5064(7)	0.5	0.131(6)
O(7SA)	0.2208(8)	0.5919(11)	0.4549(6)	0.51(1)	0.064(4)
O(8SA)	0.2939(9)	0.5908(11)	0.3966(6)	0.51(1)	0.089(5)
O(7SB)	0.2027(9)	0.7252(11)	0.4571(6)	0.49(1)	0.083(5)
O(8SB)	0.2236(11)	0.5672(14)	0.4348(8)	0.49(1)	0.094(6)
O(1W)	0.5090(18)	-0.087(2)	0.3411(12)	0.30(2)	0.118(14)
N(1)	0.2762(3)	0.5833(3)	0.19448(19)	1	0.0284(11)
N(2)	0.3277(3)	0.5120(4)	0.1078(2)	1	0.0326(11)
N(3)	0.4473(3)	0.7058(4)	0.1741(2)	1	0.0310(11)
N(4)	0.3081(3)	0.7797(3)	0.1120(2)	1	0.0287(11)
N(5)	0.5845(3)	0.8258(4)	0.2138(3)	1	0.0493(16)
N(6)	0.5719(3)	1.0296(4)	0.1918(2)	1	0.0425(14)
N(7)	0.2923(3)	0.9823(4)	0.0901(2)	1	0.0319(11)
N(8)	0.4243(3)	1.1034(4)	0.1246(2)	1	0.0315(11)
N(9)	0.2534(3)	0.1828(3)	0.1500(2)	1	0.0285(11)
N(10)	0.3218(3)	0.3084(4)	0.0855(2)	1	0.0407(13)
N(11)	0.2513(3)	1.1528(3)	-0.0023(2)	1	0.0306(11)
N(12)	0.1221(3)	1.1275(4)	0.0481(2)	1	0.0340(12)

Atom	*x*/*a*	*y*/*b*	*z*/*c*	s.o.f.	U_{eq}
N(13)	-0.0396(3)	1.1250(4)	-0.0157(2)	1	0.0376(12)
N(14)	-0.0701(3)	1.1305(4)	-0.1298(2)	1	0.0425(14)
N(15)	0.0633(3)	1.1519(4)	-0.1792(2)	1	0.0313(11)
N(16)	0.2167(3)	1.1636(4)	-0.1177(2)	1	0.0341(12)
N(17)	0.2113(3)	0.4558(4)	0.2618(2)	1	0.0310(11)
N(18)	0.2019(3)	0.2607(3)	0.2414(2)	1	0.0299(11)
N(1S)	0.1637(9)	0.0609(11)	0.4136(6)	0.72(1)	0.100(5)
N(2S)	0.3652(9)	0.0788(11)	0.3931(6)	0.64(1)	0.089(4)
N(3S)	0.4609(6)	0.5065(7)	0.4807(4)	0.5	0.086(3)
N(4SA)	0.2541(9)	0.6384(11)	0.4214(6)	0.51(1)	0.047(3)
N(4SB)	0.2331(12)	0.6587(15)	0.4372(8)	0.49(1)	0.072(5)
C(1)	0.2474(4)	0.6164(4)	0.2365(3)	1	0.0325(14)
H(1)	0.2484	0.6838	0.2435	1	0.039
C(2)	0.2705(3)	0.4854(4)	0.1851(2)	1	0.0260(12)
C(3)	0.2984(3)	0.4468(4)	0.1390(2)	1	0.0278(12)
C(4)	0.2945(4)	0.3463(4)	0.1279(2)	1	0.0300(13)
C(5)	0.3495(5)	0.3728(5)	0.0548(3)	1	0.0511(19)
H(5)	0.3683	0.3496	0.0250	1	0.061
C(6)	0.3522(4)	0.4746(5)	0.0649(3)	1	0.0441(17)
H(6)	0.3713	0.5167	0.0413	1	0.053
C(7)	0.5162(4)	0.6693(5)	0.2035(3)	1	0.0439(17)
H(7)	0.5200	0.6023	0.2118	1	0.053
C(8)	0.5832(4)	0.7300(6)	0.2224(4)	1	0.060(2)
H(8)	0.6312	0.7009	0.2426	1	0.073
C(9)	0.2389(3)	0.8199(4)	0.0827(2)	1	0.0327(14)
H(9)	0.1942	0.7793	0.0685	1	0.039
C(10)	0.2316(4)	0.9204(4)	0.0728(3)	1	0.0354(14)
H(10)	0.1814	0.9450	0.0531	1	0.043
C(11)	0.3707(3)	0.8441(4)	0.1301(2)	1	0.0242(12)
C(12)	0.4460(3)	0.8035(4)	0.1635(2)	1	0.0274(12)
C(13)	0.5133(4)	0.8640(4)	0.1835(3)	1	0.0363(14)
C(14)	0.5077(4)	0.9698(4)	0.1714(2)	1	0.0305(13)
C(15)	0.4334(3)	1.0075(4)	0.1388(2)	1	0.0256(12)
C(16)	0.3647(3)	0.9436(4)	0.1191(2)	1	0.0247(12)
C(17)	0.5607(4)	1.1238(5)	0.1775(3)	1	0.0452(17)
H(17)	0.6033	1.1679	0.1909	1	0.054
C(18)	0.4885(4)	1.1600(5)	0.1437(3)	1	0.0392(15)
H(18)	0.4855	1.2264	0.1341	1	0.047
C(19)	0.0582(4)	1.1198(5)	0.0703(3)	1	0.0385(15)
H(19)	0.0672	1.1144	0.1084	1	0.046
C(20)	-0.0213(4)	1.1195(5)	0.0386(3)	1	0.0380(15)
H(20)	-0.0640	1.1153	0.0564	1	0.046
C(21)	0.3092(4)	1.1653(5)	-0.0293(3)	1	0.0402(15)
H(21)	0.3633	1.1711	-0.0092	1	0.048

Atom	*x*/*a*	*y*/*b*	*z*/*c*	s.o.f.	U_{eq}
C(22)	0.2927(4)	1.1703(5)	-0.0868(3)	1	0.0406(15)
H(22)	0.3360	1.1784	-0.1038	1	0.049
C(23)	0.1055(3)	1.1354(4)	-0.0073(2)	1	0.0273(12)
C(24)	0.1734(3)	1.1455(4)	-0.0333(2)	1	0.0273(12)
C(25)	0.1573(3)	1.1521(4)	-0.0904(2)	1	0.0281(12)
C(26)	0.0740(3)	1.1470(4)	-0.1236(2)	1	0.0291(13)
C(27)	0.0081(3)	1.1367(4)	-0.0993(2)	1	0.0318(13)
C(28)	0.0246(3)	1.1319(4)	-0.0398(3)	1	0.0313(13)
C(29)	-0.0789(4)	1.1358(5)	-0.1834(3)	1	0.0465(18)
H(29)	-0.1317	1.1322	-0.2059	1	0.056
C(30)	-0.0131(4)	1.1467(5)	-0.2088(3)	1	0.0391(15)
H(30)	-0.0235	1.1503	-0.2471	1	0.047
C(31)	0.2159(3)	0.5529(4)	0.2704(3)	1	0.0314(13)
H(31)	0.1976	0.5790	0.2998	1	0.038
C(32)	0.2389(3)	0.4224(4)	0.2186(2)	1	0.0273(12)
C(33)	0.2335(3)	0.3185(4)	0.2072(2)	1	0.0258(12)
C(34)	0.2601(3)	0.2808(4)	0.1620(2)	1	0.0278(13)
C(35)	0.1970(4)	0.1651(5)	0.2292(3)	1	0.0356(14)
H(35)	0.1767	0.1221	0.2518	1	0.043
C(36)	0.2217(4)	0.1271(5)	0.1833(3)	1	0.0347(14)
H(36)	0.2156	0.0599	0.1760	1	0.042
C(37)	0.0611(5)	0.5648(9)	0.1362(4)	1	0.079(3)
H(37)	0.0507	0.6079	0.1627	1	0.094
C(38)	0.0520(6)	0.4670(11)	0.1422(5)	1	0.095(4)
H(38)	0.0344	0.4441	0.1725	1	0.114
C(39)	0.0673(7)	0.4024(9)	0.1062(6)	1	0.097(4)
H(39)	0.0615	0.3354	0.1120	1	0.117
C(40)	0.0920(7)	0.4339(11)	0.0601(6)	1	0.108(5)
H(40)	0.1017	0.3893	0.0341	1	0.130
C(41)	0.1020(6)	0.5369(11)	0.0539(5)	1	0.091(3)
H(41)	0.1200	0.5612	0.0239	1	0.110
C(42)	0.0849(5)	0.6004(7)	0.0925(5)	1	0.076(3)
H(42)	0.0898	0.6681	0.0884	1	0.092
C(1S)	0.1492(14)	0.0689(17)	0.3600(9)	0.72(1)	0.155(9)
H(1S1)	0.1359	0.0053	0.3435	0.72(1)	0.232
H(1S2)	0.1971	0.0944	0.3500	0.72(1)	0.232
H(1S3)	0.1039	0.1131	0.3472	0.72(1)	0.232
C(2S)	0.4285(11)	-0.0056(13)	0.4001(7)	0.64(1)	0.100(6)
H(2S1)	0.4140	-0.0563	0.4228	0.64(1)	0.151
H(2S2)	0.4821	0.0194	0.4171	0.64(1)	0.151
H(2S3)	0.4288	-0.0325	0.3645	0.64(1)	0.151
C(3S)	0.4609(6)	0.5065(7)	0.4807(4)	0.5	0.086(3)
C(4SA)	0.2482(14)	0.7437(17)	0.4145(9)	0.51(1)	0.093(7)
H(4S4)	0.3005	0.7732	0.4306	0.51(1)	0.139

Atom	*x*/*a*	*y*/*b*	*z*/*c*	s.o.f.	U_{eq}
H(4S5)	0.2077	0.7689	0.4324	0.51(1)	0.139
H(4S6)	0.2325	0.7593	0.3759	0.51(1)	0.139
C(4SB)	0.2945(12)	0.6946(15)	0.4032(8)	0.49(1)	0.070(6)
H(4S1)	0.2761	0.7566	0.3860	0.49(1)	0.104
H(4S2)	0.2970	0.6468	0.3753	0.49(1)	0.104
H(4S3)	0.3480	0.7025	0.4272	0.49(1)	0.104
B(1)	0.3205(6)	0.9047(7)	0.2621(4)	1	0.055(2)
B(2)	-0.0344(5)	0.1489(7)	0.1937(4)	1	0.054(2)
B(3A)	0.5347(10)	0.2627(11)	-0.0172(6)	0.61(1)	0.039(4)
B(3B)	0.507(2)	0.283(3)	-0.0255(14)	0.39(1)	0.065(9)

Table 1B. Bond distances (Å) in the crystal structure of **1**.

Cu(1)–N(4)	1.967(5)	O(2S)–N(1S)	1.141(15)
Cu(1)–N(2)	1.979(5)	O(3S)–N(2S)	1.261(17)
Cu(1)–N(3)	2.034(5)	O(4S)–N(2S)	1.158(16)
Cu(1)–N(1)	2.038(5)	O(5S)–N(3S)	1.109(14)
Cu(2)–N(11)	2.007(5)	O(6S)–N(3S)	1.333(14)
Cu(2)–N(7)	2.056(5)	O(7SA)–N(4SA)	1.28(2)
Cu(2)–N(9)	2.057(5)	O(8SA)–N(4SA)	1.202(19)
Cu(2)–N(8)	2.388(5)	O(7SB)–N(4SB)	1.20(2)
Cu(2)–N(10)	2.462(6)	O(8SB)–N(4SB)	1.25(3)
Cu(3)–N(18)	1.986(5)	N(1)–C(1)	1.333(7)
Cu(3)–N(15)	1.998(5)	N(1)–C(2)	1.348(7)
Cu(3)–N(16)	2.008(5)	N(2)–C(6)	1.337(8)
Cu(3)–N(17)	2.040(5)	N(2)–C(3)	1.345(7)
F(1)–B(1)	1.366(10)	N(3)–C(7)	1.310(8)
F(2)–B(1)	1.353(11)	N(3)–C(12)	1.352(7)
F(3)–B(1)	1.269(12)	N(4)–C(9)	1.332(7)
F(4)–B(1)	1.364(11)	N(4)–C(11)	1.357(7)
F(5)–B(2)	1.367(10)	N(5)–C(8)	1.318(9)
F(6)–B(2)	1.393(11)	N(5)–C(13)	1.355(8)
F(7)–B(2)	1.319(12)	N(6)–C(17)	1.328(8)
F(8)–B(2)	1.317(10)	N(6)–C(14)	1.347(8)
F(9A)–B(3A)	1.366(18)	N(7)–C(10)	1.311(8)
F(10A)–B(3A)	1.332(17)	N(7)–C(16)	1.362(7)
F(11A)–B(3A)	1.433(18)	N(8)–C(18)	1.316(8)
F(12A)–B(3A)	1.383(19)	N(8)–C(15)	1.347(7)
F(9B)–B(3B)	1.34(4)	N(9)–C(36)	1.325(8)
F(10B)–B(3B)	1.49(4)	N(9)–C(34)	1.361(7)
F(11B)–B(3B)	1.31(4)	N(10)–C(5)	1.318(9)
F(12B)–B(3B)	1.44(4)	N(10)–C(4)	1.350(8)
O(1S)–N(1S)	1.27(2)	N(11)–C(21)	1.317(8)

N(11)–C(24)	1.355(7)	N(1S)–C(1S)	1.31(2)
N(12)–C(19)	1.324(8)	N(2S)–C(2S)	1.54(2)
N(12)–C(23)	1.349(8)	N(3S)–C(3S)	1.440(18)
N(13)–C(20)	1.319(8)	N(4SA)–C(4SA)	1.44(3)
N(13)–C(28)	1.357(7)	N(4SB)–C(4SB)	1.56(3)
N(14)–C(29)	1.312(9)	C(1)–C(31)	1.398(9)
N(14)–C(27)	1.353(8)	C(2)–C(32)	1.386(8)
N(15)–C(30)	1.318(8)	C(2)–C(3)	1.440(8)
N(15)–C(26)	1.360(7)	C(3)–C(4)	1.390(8)
N(16)–C(22)	1.325(8)	C(4)–C(34)	1.444(8)
N(16)–C(25)	1.344(7)	C(5)–C(6)	1.401(10)
N(17)–C(31)	1.333(8)	C(7)–C(8)	1.382(10)
N(17)–C(32)	1.348(7)	C(9)–C(10)	1.386(8)
N(18)–C(35)	1.330(8)	C(11)–C(16)	1.376(8)
N(18)–C(33)	1.355(7)	C(11)–C(12)	1.445(8)

Table 1C. Bond angles (°) in the crystal structure of **1**.

N(4)–Cu(1)–N(2)	135.4(2)	C(3)–N(2)–Cu(1)	111.2(4)
N(4)–Cu(1)–N(3)	83.7(2)	C(7)–N(3)–C(12)	116.8(5)
N(2)–Cu(1)–N(3)	120.0(2)	C(7)–N(3)–Cu(1)	133.1(4)
N(4)–Cu(1)–N(1)	120.94(19)	C(12)–N(3)–Cu(1)	110.1(4)
N(2)–Cu(1)–N(1)	84.2(2)	C(9)–N(4)–C(11)	115.0(5)
N(3)–Cu(1)–N(1)	116.1(2)	C(9)–N(4)–Cu(1)	132.4(4)
N(11)–Cu(2)–N(7)	104.91(19)	C(11)–N(4)–Cu(1)	112.4(4)
N(11)–Cu(2)–N(9)	139.71(19)	C(8)–N(5)–C(13)	114.9(6)
N(7)–Cu(2)–N(9)	104.1(2)	C(17)–N(6)–C(14)	115.4(6)
N(11)–Cu(2)–N(8)	119.95(19)	C(10)–N(7)–C(16)	116.8(5)
N(7)–Cu(2)–N(8)	75.22(17)	C(10)–N(7)–Cu(2)	124.7(4)
N(9)–Cu(2)–N(8)	94.13(18)	C(16)–N(7)–Cu(2)	118.4(4)
N(11)–Cu(2)–N(10)	86.10(18)	C(18)–N(8)–C(15)	115.9(5)
N(7)–Cu(2)–N(10)	160.64(19)	C(18)–N(8)–Cu(2)	134.6(4)
N(9)–Cu(2)–N(10)	75.10(18)	C(15)–N(8)–Cu(2)	108.8(4)
N(8)–Cu(2)–N(10)	85.50(18)	C(36)–N(9)–C(34)	116.3(5)
N(18)–Cu(3)–N(15)	129.1(2)	C(36)–N(9)–Cu(2)	124.4(4)
N(18)–Cu(3)–N(16)	129.8(2)	C(34)–N(9)–Cu(2)	119.2(4)
N(15)–Cu(3)–N(16)	83.5(2)	C(5)–N(10)–C(4)	115.8(5)
N(18)–Cu(3)–N(17)	84.0(2)	C(5)–N(10)–Cu(2)	136.9(5)
N(15)–Cu(3)–N(17)	119.9(2)	C(4)–N(10)–Cu(2)	106.5(4)
N(16)–Cu(3)–N(17)	114.3(2)	C(21)–N(11)–C(24)	116.3(5)
C(1)–N(1)–C(2)	116.4(5)	C(21)–N(11)–Cu(2)	119.0(4)
C(1)–N(1)–Cu(1)	134.9(4)	C(24)–N(11)–Cu(2)	124.3(4)
C(2)–N(1)–Cu(1)	108.6(4)	C(19)–N(12)–C(23)	116.5(5)
C(6)–N(2)–C(3)	116.0(5)	C(20)–N(13)–C(28)	116.5(5)
C(6)–N(2)–Cu(1)	132.5(5)	C(29)–N(14)–C(27)	115.4(6)

C(30)–N(15)–C(26)	116.4(5)	N(3)–C(12)–C(13)	122.4(5)
C(30)–N(15)–Cu(3)	132.6(4)	N(3)–C(12)–C(11)	117.2(5)
C(26)–N(15)–Cu(3)	110.9(4)	C(13)–C(12)–C(11)	120.4(5)
C(22)–N(16)–C(25)	116.1(5)	N(5)–C(13)–C(12)	120.5(6)
C(22)–N(16)–Cu(3)	132.3(4)	N(5)–C(13)–C(14)	119.6(5)
C(25)–N(16)–Cu(3)	111.5(4)	C(12)–C(13)–C(14)	119.9(5)
C(31)–N(17)–C(32)	116.4(5)	N(6)–C(14)–C(15)	121.0(5)
C(31)–N(17)–Cu(3)	134.2(4)	N(6)–C(14)–C(13)	120.4(5)
C(32)–N(17)–Cu(3)	109.4(4)	C(15)–C(14)–C(13)	118.5(5)
C(35)–N(18)–C(33)	115.7(5)	N(8)–C(15)–C(14)	122.1(5)
C(35)–N(18)–Cu(3)	133.1(4)	N(8)–C(15)–C(16)	117.5(5)
C(33)–N(18)–Cu(3)	111.2(4)	C(14)–C(15)–C(16)	120.4(5)
O(2S)–N(1S)–O(1S)	118.2(18)	N(7)–C(16)–C(11)	119.9(5)
O(2S)–N(1S)–C(1S)	122.6(18)	N(7)–C(16)–C(15)	119.4(5)
O(1S)–N(1S)–C(1S)	118(2)	C(11)–C(16)–C(15)	120.7(5)
O(4S)–N(2S)–O(3S)	118.0(16)	N(6)–C(17)–C(18)	123.4(6)
O(4S)–N(2S)–C(2S)	128.9(16)	N(8)–C(18)–C(17)	122.1(6)
O(3S)–N(2S)–C(2S)	112.6(14)	N(12)–C(19)–C(20)	121.9(6)
O(5S)–N(3S)–O(6S)	116.4(14)	N(13)–C(20)–C(19)	123.1(6)
O(5S)–N(3S)–C(3S)	132.2(15)	N(11)–C(21)–C(22)	122.9(6)
O(6S)–N(3S)–C(3S)	111.3(14)	N(16)–C(22)–C(21)	121.4(6)
O(8SA)–N(4SA)–O(7SA)	117.1(16)	N(12)–C(23)–C(28)	121.7(5)
O(8SA)–N(4SA)–C(4SA)	120.2(17)	N(12)–C(23)–C(24)	118.5(5)
O(7SA)–N(4SA)–C(4SA)	123(2)	C(28)–C(23)–C(24)	119.9(5)
O(7SB)–N(4SB)–O(8SB)	135(2)	N(11)–C(24)–C(25)	120.5(5)
O(7SB)–N(4SB)–C(4SB)	113.0(18)	N(11)–C(24)–C(23)	120.3(5)
O(8SB)–N(4SB)–C(4SB)	112(2)	C(25)–C(24)–C(23)	119.1(5)
N(1)–C(1)–C(31)	122.0(5)	N(16)–C(25)–C(24)	122.8(5)
N(1)–C(2)–C(32)	121.6(5)	N(16)–C(25)–C(26)	116.6(5)
N(1)–C(2)–C(3)	118.3(5)	C(24)–C(25)–C(26)	120.7(5)
C(32)–C(2)–C(3)	120.2(5)	N(15)–C(26)–C(27)	121.8(5)
N(2)–C(3)–C(4)	122.4(5)	N(15)–C(26)–C(25)	117.2(5)
N(2)–C(3)–C(2)	117.2(5)	C(27)–C(26)–C(25)	121.0(5)
C(4)–C(3)–C(2)	120.4(5)	N(14)–C(27)–C(26)	121.7(6)
N(10)–C(4)–C(3)	121.4(5)	N(14)–C(27)–C(28)	119.9(5)
N(10)–C(4)–C(34)	119.1(5)	C(26)–C(27)–C(28)	118.4(5)
C(3)–C(4)–C(34)	119.5(5)	N(13)–C(28)–C(23)	120.3(6)
N(10)–C(5)–C(6)	123.3(6)	N(13)–C(28)–C(27)	118.8(5)
N(2)–C(6)–C(5)	121.0(6)	C(23)–C(28)–C(27)	121.0(5)
N(3)–C(7)–C(8)	120.2(6)	N(14)–C(29)–C(30)	123.8(6)
N(5)–C(8)–C(7)	125.1(6)	N(15)–C(30)–C(29)	120.9(6)
N(4)–C(9)–C(10)	121.9(5)	N(17)–C(31)–C(1)	121.7(5)
N(7)–C(10)–C(9)	122.9(5)	N(17)–C(32)–C(2)	121.9(5)
N(4)–C(11)–C(16)	123.4(5)	N(17)–C(32)–C(33)	118.1(5)
N(4)–C(11)–C(12)	116.5(5)	C(2)–C(32)–C(33)	120.0(5)
C(16)–C(11)–C(12)	120.1(5)	N(18)–C(33)–C(34)	122.7(5)

N(18)–C(33)–C(32)	117.3(5)	F(8)–B(2)–F(7)	113.4(9)
C(34)–C(33)–C(32)	119.9(5)	F(8)–B(2)–F(5)	115.2(7)
N(9)–C(34)–C(33)	120.6(5)	F(7)–B(2)–F(5)	111.9(8)
N(9)–C(34)–C(4)	119.6(5)	F(8)–B(2)–F(6)	107.2(8)
C(33)–C(34)–C(4)	119.9(5)	F(7)–B(2)–F(6)	103.7(8)
N(18)–C(35)–C(36)	121.9(6)	F(5)–B(2)–F(6)	104.1(8)
N(9)–C(36)–C(35)	122.8(6)	F(10A)–B(3A)–F(9A)	116.5(12)
C(42)–C(37)–C(38)	120.6(11)	F(10A)–B(3A)–F(12A)	109.7(12)
C(39)–C(38)–C(37)	122.1(12)	F(9A)–B(3A)–F(12A)	110.7(13)
C(38)–C(39)–C(40)	120.5(12)	F(10A)–B(3A)–F(11A)	104.3(12)
C(39)–C(40)–C(41)	117.6(11)	F(9A)–B(3A)–F(11A)	103.4(12)
C(42)–C(41)–C(40)	119.3(11)	F(12A)–B(3A)–F(11A)	111.9(12)
C(37)–C(42)–C(41)	120.0(10)	F(11B)–B(3B)–F(9B)	129(3)
F(3)–B(1)–F(2)	112.3(8)	F(11B)–B(3B)–F(12B)	120(3)
F(3)–B(1)–F(4)	108.1(10)	F(9B)–B(3B)–F(12B)	96(2)
F(2)–B(1)–F(4)	106.7(8)	F(11B)–B(3B)–F(10B)	105(2)
F(3)–B(1)–F(1)	115.0(10)	F(9B)–B(3B)–F(10B)	98(2)
F(2)–B(1)–F(1)	108.6(7)	F(12B)–B(3B)–F(10B)	105(2)
F(4)–B(1)–F(1)	105.5(7)		

Table 2A. Positional and thermal parameters for **2**.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Cu(1)	0.85266(5)	0.85266(5)	0.0000	1	0.0219(3)
P(1)	1.3565(10)	0.9545(13)	-0.0181(11)	0.5	0.260(12)
F(1)	1.4891(14)	0.919(2)	-0.023(3)	0.5	0.77(11)
F(2)	1.323(2)	0.827(2)	-0.052(3)	0.5	0.50(2)
F(3)	1.360(2)	0.978(3)	-0.1404(16)	0.5	0.39(4)
F(4)	1.391(2)	1.0864(15)	-0.003(3)	0.5	0.35(3)
F(5)	1.362(3)	0.9394(19)	0.1061(17)	0.5	0.57(7)
F(6)	1.2242(14)	0.986(3)	-0.0097(14)	0.5	0.202(14)
N(1)	1.0005(4)	0.8013(4)	0.0710(3)	1	0.0186(8)
N(2)	0.7029(4)	0.7928(4)	0.0890(3)	1	0.0220(9)
N(3)	0.8966(4)	0.9943(4)	0.1645(4)	1	0.0264(10)
C(1)	1.0556(5)	0.7101(5)	0.0307(4)	1	0.0227(10)
H(1)	1.0257	0.6762	-0.0298	1	0.027
C(2)	1.1564(6)	0.6626(5)	0.0749(4)	1	0.0274(11)
H(2)	1.1913	0.5987	0.0432	1	0.033
C(3)	1.1488(5)	0.8010(4)	0.2028(3)	1	0.0184(9)
C(4)	1.0490(4)	0.8475(5)	0.1591(4)	1	0.0179(8)
C(5)	0.9963(4)	0.9501(4)	0.2066(4)	1	0.0192(9)
C(6)	0.8553(6)	1.0896(5)	0.2067(5)	1	0.0308(12)
H(6)	0.7879	1.1223	0.1792	1	0.037

Table 2B. Bond distances (Å) in the crystal structure of **2**.

Cu(1)–N(1)	2.014(4)	N(2)–C(2)	1.324(7)
Cu(1)–N(1)	2.014(4)	N(2)–C(3)	1.354(6)
Cu(1)–N(2)	2.173(5)	N(3)–C(6)	1.309(7)
Cu(1)–N(2)	2.173(5)	N(3)–C(5)	1.365(7)
P(1)–F(6)	1.566(15)	C(1)–C(2)	1.400(8)
P(1)–F(4)	1.578(15)	C(2)–N(2)	1.324(7)
P(1)–F(1)	1.579(15)	C(3)–N(2)	1.354(6)
P(1)–F(3)	1.582(14)	C(3)–C(4)	1.384(7)
P(1)–F(2)	1.583(16)	C(3)–C(3)	1.452(9)
P(1)–F(5)	1.592(16)	C(4)–C(5)	1.457(7)
N(1)–C(1)	1.329(7)	C(5)–C(5)	1.407(9)
N(1)–C(4)	1.360(6)	C(6)–C(6)	1.420(11)

Table 2C. Bond angles (°) in the crystal structure of **2**.

N(1)–Cu(1)–N(1)	134.1(2)	F(2)–P(1)–F(5)	100.5(18)
N(1)–Cu(1)–N(2)	109.97(17)	C(1)–N(1)–C(4)	115.5(4)
N(1)–Cu(1)–N(2)	105.64(18)	C(1)–N(1)–Cu(1)	117.4(3)
N(1)–Cu(1)–N(2)	105.64(18)	C(4)–N(1)–Cu(1)	127.0(4)
N(1)–Cu(1)–N(2)	109.97(17)	C(2)–N(2)–C(3)	116.7(5)
N(2)–Cu(1)–N(2)	76.7(2)	C(2)–N(2)–Cu(1)	129.0(4)
F(6)–P(1)–F(4)	90.8(11)	C(3)–N(2)–Cu(1)	114.3(3)
F(6)–P(1)–F(1)	177.8(12)	C(6)–N(3)–C(5)	117.1(5)
F(4)–P(1)–F(1)	90.6(9)	N(1)–C(1)–C(2)	123.2(5)
F(6)–P(1)–F(3)	93.2(9)	N(2)–C(2)–C(1)	121.1(5)
F(4)–P(1)–F(3)	87.1(9)	N(2)–C(3)–C(4)	122.1(4)
F(1)–P(1)–F(3)	88.6(10)	N(2)–C(3)–C(3)	117.3(3)
F(6)–P(1)–F(2)	89.5(9)	C(4)–C(3)–C(3)	120.6(3)
F(4)–P(1)–F(2)	170.9(19)	N(1)–C(4)–C(3)	121.4(5)
F(1)–P(1)–F(2)	89.4(11)	N(1)–C(4)–C(5)	119.2(4)
F(3)–P(1)–F(2)	84(2)	C(3)–C(4)–C(5)	119.3(4)
F(6)–P(1)–F(5)	89.9(10)	N(3)–C(5)–C(5)	120.9(3)
F(4)–P(1)–F(5)	88.5(11)	N(3)–C(5)–C(4)	119.2(4)
F(1)–P(1)–F(5)	88.5(9)	C(5)–C(5)–C(4)	119.9(3)
F(3)–P(1)–F(5)	174.6(13)	N(3)–C(6)–C(6)	122.0(3)

Table 3A. Positional and thermal parameters for **3**.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
Sb(1)	0.70253(5)	0.24740(6)	0.45985(2)	0.0456(2)
Sb(2)	0.48203(5)	0.67118(4)	0.391641(18)	0.03264(14)
Sb(3)	0.28518(5)	0.25177(6)	0.13907(2)	0.0462(2)
Sb(4)	0.06176(5)	-0.16760(5)	0.209493(19)	0.03651(16)
Cu(1)	0.23032(8)	-0.24819(8)	0.50903(3)	0.0314(3)
Cu(2)	0.48084(8)	0.03310(8)	0.39023(4)	0.0342(2)
Cu(3)	0.55248(8)	0.03204(8)	0.21011(4)	0.0334(3)
Cu(4)	0.30839(7)	-0.25459(8)	0.09123(3)	0.0291(3)
F(1)	0.7516(9)	0.1391(8)	0.4811(3)	0.124(4)
F(2)	0.8278(7)	0.3035(10)	0.4592(3)	0.127(5)
F(3)	0.6820(7)	0.3001(8)	0.5046(2)	0.099(3)
F(4)	0.5753(6)	0.1946(8)	0.4600(3)	0.097(3)
F(5)	0.7246(10)	0.1914(8)	0.4156(2)	0.121(4)
F(6)	0.6543(9)	0.3521(7)	0.4381(4)	0.134(5)
F(7)	0.5826(5)	0.5824(5)	0.38441(18)	0.0589(19)
F(8)	0.4877(4)	0.6497(5)	0.44105(18)	0.0518(18)
F(9)	0.5777(7)	0.7652(7)	0.3974(2)	0.099(4)
F(10)	0.4753(6)	0.6980(6)	0.34273(19)	0.064(2)
F(11)	0.3891(4)	0.5733(5)	0.38668(17)	0.0533(16)
F(12)	0.3772(7)	0.7539(6)	0.4015(2)	0.087(3)
F(13)	0.4131(7)	0.2024(10)	0.1381(3)	0.139(6)
F(14)	0.3028(11)	0.2982(15)	0.1845(3)	0.190(8)
F(15)	0.3416(12)	0.3553(8)	0.1200(5)	0.196(8)
F(16)	0.2708(7)	0.2139(11)	0.0933(2)	0.130(5)
F(17)	0.2356(19)	0.1506(10)	0.1602(6)	0.246(12)
F(18)	0.1606(6)	0.3024(9)	0.1381(3)	0.123(5)
F(19)	0.1652(10)	-0.2512(7)	0.2028(3)	0.125(5)
F(20)	0.1504(5)	-0.0698(6)	0.2118(2)	0.083(3)
F(21)	0.0666(7)	-0.1815(7)	0.25846(19)	0.081(3)
F(22)	-0.0270(10)	-0.2663(7)	0.2059(3)	0.126(5)
F(23)	0.0553(5)	-0.1531(5)	0.15938(18)	0.0521(19)
F(24)	-0.0411(4)	-0.0807(5)	0.21415(19)	0.059(2)
N(1)	0.2756(5)	-0.1391(5)	0.4728(2)	0.0244(15)
N(2)	0.3754(5)	-0.2419(5)	0.5228(2)	0.0256(15)
N(3)	0.5842(5)	-0.2440(5)	0.5227(2)	0.0263(15)
N(4)	0.6868(5)	-0.1436(5)	0.47261(19)	0.0262(16)
N(5)	0.5826(5)	-0.0290(5)	0.42344(19)	0.0242(15)
N(6)	0.3809(5)	-0.0287(5)	0.4228(2)	0.0274(16)
N(7)	0.4984(6)	0.0035(5)	0.33697(19)	0.0298(16)
N(8)	0.4749(5)	0.1665(5)	0.3728(2)	0.0240(16)
N(9)	0.4653(5)	0.3381(5)	0.3351(2)	0.0310(17)
N(10)	0.4991(6)	0.3374(5)	0.2616(2)	0.0305(17)

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
N(11)	0.5352(5)	0.1670(5)	0.2268(2)	0.0258(16)
N(12)	0.5310(5)	0.0026(5)	0.2624(2)	0.0268(15)
N(13)	0.4508(5)	-0.0316(5)	0.1763(2)	0.0251(15)
N(14)	0.6543(5)	-0.0327(5)	0.17862(18)	0.0231(15)
N(15)	0.7631(5)	-0.1393(5)	0.12831(18)	0.0256(15)
N(16)	0.6650(5)	-0.2409(5)	0.07793(19)	0.0232(15)
N(17)	0.4519(5)	-0.2454(5)	0.0780(2)	0.0259(16)
N(18)	0.3489(5)	-0.1443(5)	0.1270(2)	0.0289(17)
C(1)	0.4277(7)	-0.2866(9)	0.5469(3)	0.042(3)
H(1)	0.3943	-0.3180	0.5651	0.051
C(2)	0.5326(7)	-0.2888(8)	0.5462(3)	0.043(3)
H(2)	0.5661	-0.3238	0.5634	0.052
C(3)	0.7325(7)	-0.0920(7)	0.4478(2)	0.032(2)
H(3)	0.8019	-0.0934	0.4468	0.038
C(4)	0.6819(7)	-0.0363(6)	0.4235(3)	0.034(2)
H(4)	0.7184	-0.0030	0.4066	0.041
C(5)	0.2807(6)	-0.0340(6)	0.4240(2)	0.030(2)
H(5)	0.2443	0.0000	0.4073	0.036
C(6)	0.2284(6)	-0.0875(7)	0.4490(2)	0.031(2)
H(6)	0.1589	-0.0869	0.4488	0.037
C(7)	0.4295(5)	-0.1910(6)	0.4995(2)	0.0219(17)
C(8)	0.5327(5)	-0.1912(6)	0.4992(2)	0.0206(16)
C(9)	0.5860(6)	-0.1364(6)	0.4724(2)	0.0194(16)
C(10)	0.5347(6)	-0.0820(6)	0.4488(2)	0.0247(18)
C(11)	0.4273(6)	-0.0814(6)	0.4482(2)	0.0183(16)
C(12)	0.3735(6)	-0.1348(5)	0.4730(2)	0.0190(15)
C(13)	0.5131(7)	-0.0758(6)	0.3192(2)	0.036(2)
H(13)	0.5138	-0.1323	0.3317	0.043
C(14)	0.5276(8)	-0.0768(7)	0.2822(3)	0.045(2)
H(14)	0.5353	-0.1343	0.2708	0.054
C(15)	0.5374(7)	0.2477(6)	0.2093(3)	0.036(2)
H(15)	0.5534	0.2483	0.1852	0.043
C(16)	0.5158(8)	0.3322(8)	0.2267(3)	0.040(2)
H(16)	0.5131	0.3870	0.2133	0.048
C(17)	0.4500(8)	0.3325(7)	0.3701(3)	0.038(2)
H(17)	0.4346	0.3872	0.3825	0.046
C(18)	0.4559(6)	0.2484(7)	0.3891(3)	0.034(2)
H(18)	0.4464	0.2492	0.4137	0.040
C(19)	0.5021(6)	0.0846(6)	0.3183(2)	0.0249(16)
C(20)	0.5181(6)	0.0842(6)	0.2819(2)	0.0246(16)
C(21)	0.5191(5)	0.1718(6)	0.2630(2)	0.0236(17)
C(22)	0.5012(5)	0.2554(6)	0.2793(2)	0.0242(17)
C(23)	0.4826(6)	0.2565(5)	0.3180(2)	0.0246(16)
C(24)	0.4864(5)	0.1714(5)	0.3370(2)	0.0184(15)

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
C(25)	0.3518(7)	-0.0347(8)	0.1754(3)	0.045(3)
H(25)	0.3148	0.0021	0.1911	0.054
C(26)	0.3015(7)	-0.0942(7)	0.1505(3)	0.038(2)
H(26)	0.2321	-0.0971	0.1511	0.046
C(27)	0.5069(7)	-0.2902(8)	0.0523(3)	0.037(2)
H(27)	0.4746	-0.3250	0.0348	0.045
C(28)	0.6118(7)	-0.2840(8)	0.0522(2)	0.038(2)
H(28)	0.6463	-0.3113	0.0333	0.045
C(29)	0.8066(6)	-0.0903(7)	0.1540(2)	0.032(2)
H(29)	0.8759	-0.0915	0.1558	0.038
C(30)	0.7528(7)	-0.0372(7)	0.1786(2)	0.033(2)
H(30)	0.7877	-0.0033	0.1958	0.039
C(31)	0.5000(6)	-0.0825(6)	0.1520(2)	0.0229(18)
C(32)	0.4496(6)	-0.1398(5)	0.1275(2)	0.0200(16)
C(33)	0.5033(5)	-0.1945(6)	0.1015(2)	0.0171(16)
C(34)	0.6093(5)	-0.1918(5)	0.10184(19)	0.0175(15
C(35)	0.6619(6)	-0.1372(6)	0.1281(2)	0.0223(17)
C(36)	0.6087(6)	-0.0825(6)	0.1529(2)	0.0209(16)
C(1S)	0.3636(8)	-0.4985(11)	0.5360(4)	0.165(10)
H(1S)	0.2988	-0.4980	0.5271	0.198
C(2S)	0.3798(10)	-0.4984(11)	0.5726(4)	0.128(7)
H(2S)	0.3257	-0.4978	0.5882	0.154
C(3S)	0.4766(12)	-0.4992(12)	0.5860(4)	0.139(6)
H(3S)	0.4874	-0.4992	0.6105	0.167
C(4S)	0.5574(9)	-0.5001(14)	0.5626(4)	0.139(6)
H(4S)	0.6222	-0.5007	0.5716	0.167
C(5S)	0.5412(9)	-0.5002(12)	0.5260(4)	0.116(7)
H(5S)	0.5952	-0.5008	0.5104	0.140
C(6S)	0.4444(10)	-0.4994(10)	0.5127(4)	0.095(5)
H(6S)	0.4336	-0.4995	0.4881	0.114
C(7S)	0.7404(7)	0.4454(6)	0.2849(3)	0.076(4)
H(7S)	0.7426	0.5045	0.2744	0.091
C(8S)	0.7570(7)	0.3657(8)	0.2644(2)	0.077(4)
H(8S)	0.7702	0.3715	0.2401	0.092
C(9S)	0.7537(6)	0.2774(6)	0.2801(3)	0.084(5)
H(9S)	0.7648	0.2241	0.2663	0.101
C(10S)	0.7339(7)	0.2687(6)	0.3163(3)	0.071(4)
H(10S)	0.7317	0.2097	0.3268	0.085
C(11S)	0.7174(6)	0.3484(8)	0.3369(2)	0.079(4)
H(11S)	0.7042	0.3426	0.3612	0.094
C(12S)	0.7207(7)	0.4367(6)	0.3212(3)	0.075(4)
H(12S)	0.7096	0.4900	0.3350	0.090
C(13S)	0.5419(6)	-0.0619(5)	0.02185(16)	0.066(4)
H(13S)	0.5441	-0.1032	0.0027	0.079

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
C(14S)	0.6301(6)	-0.0302(5)	0.03724(16)	0.063(4)
H(14S)	0.6913	-0.0502	0.0283	0.076
C(15S)	0.6268(5)	0.0315(5)	0.06595(16)	0.070(4)
H(15S)	0.6858	0.0528	0.0762	0.084
C(16S)	0.5353(5)	0.0615(4)	0.07926(14)	0.056(3)
H(16S)	0.5331	0.1028	0.0985	0.067
C(17S)	0.4471(5)	0.0297(4)	0.06386(16)	0.071(5)
H(17S)	0.3859	0.0498	0.0728	0.086
C(18S)	0.4504(6)	-0.0320(5)	0.03516(17)	0.064(4)
H(18S)	0.3914	-0.0532	0.0249	0.076
N(1S)	0.2905(4)	0.4872(3)	0.29294(14)	0.063(3)
O(1S)	0.2383(5)	0.4797(4)	0.32057(15)	0.090(3)
O(2S)	0.2631(4)	0.4541(4)	0.26360(15)	0.088(3)
C(19S)	0.3887(4)	0.5349(4)	0.29310(16)	0.045(2)
H(19A)	0.4345	0.5010	0.2782	0.068
H(19B)	0.4142	0.5369	0.3170	0.068
H(19C)	0.3812	0.5976	0.2842	0.068
N(2S)	0.2748(16)	-0.2393(14)	0.2916(5)	0.145(8)
O(3S)	0.250(2)	-0.3162(16)	0.2753(6)	0.233(10)
O(4S)	0.3279(13)	-0.1807(12)	0.2791(4)	0.150(6)
C(20S)	0.2261(16)	-0.2288(14)	0.3262(5)	0.115(7)
H(20A)	0.2640	-0.1862	0.3407	0.173
H(20B)	0.2225	-0.2888	0.3378	0.173
H(20C)	0.1599	-0.2045	0.3228	0.173

Table 3B. Bond distances (Å) in the crystal structure of **3**.

Sb(1)–F(6)	1.819(9)	Sb(3)–F(14)	1.842(11)
Sb(1)–F(1)	1.856(10)	Sb(3)–F(13)	1.852(8)
Sb(1)–F(2)	1.859(8)	Sb(4)–F(20)	1.833(7)
Sb(1)–F(3)	1.859(8)	Sb(4)–F(19)	1.844(8)
Sb(1)–F(4)	1.862(7)	Sb(4)–F(22)	1.846(7)
Sb(1)–F(5)	1.864(9)	Sb(4)–F(21)	1.847(7)
Sb(2)–F(9)	1.866(6)	Sb(4)–F(24)	1.861(6)
Sb(2)–F(7)	1.867(6)	Sb(4)–F(23)	1.891(7)
Sb(2)–F(12)	1.870(7)	Cu(1)–N(2)	2.012(7)
Sb(2)–F(10)	1.874(7)	Cu(1)–N(3)	2.024(7)
Sb(2)–F(8)	1.878(7)	Cu(1)–N(4)	2.140(8)
Sb(2)–F(11)	1.879(6)	Cu(1)–N(1)	2.151(8)
Sb(3)–F(17)	1.773(14)	Cu(2)–N(8)	2.012(7)
Sb(3)–F(15)	1.804(11)	Cu(2)–N(6)	2.014(8)
Sb(3)–F(16)	1.806(9)	Cu(2)–N(5)	2.046(8)
Sb(3)–F(18)	1.817(7)	Cu(2)–N(7)	2.053(7)

Cu(3)–N(12)	2.023(8)	N(18)–C(26)	1.298(12)
Cu(3)–N(14)	2.026(7)	N(18)–C(32)	1.350(10)
Cu(3)–N(11)	2.035(8)	C(1)–C(2)	1.406(13)
Cu(3)–N(13)	2.069(7)	C(3)–C(4)	1.385(13)
Cu(4)–N(16)	1.985(7)	C(5)–C(6)	1.395(13)
Cu(4)–N(17)	1.989(6)	C(7)–C(8)	1.382(11)
Cu(4)–N(18)	2.136(8)	C(7)–C(12)	1.479(12)
Cu(4)–N(15)	2.141(7)	C(8)–C(9)	1.457(12)
N(1)–C(12)	1.313(11)	C(9)–C(10)	1.363(12)
N(1)–C(6)	1.319(11)	C(10)–C(11)	1.439(12)
N(2)–C(1)	1.309(13)	C(11)–C(12)	1.400(11)
N(2)–C(7)	1.347(11)	C(13)–C(14)	1.400(12)
N(3)–C(2)	1.289(13)	C(15)–C(16)	1.399(15)
N(3)–C(8)	1.348(11)	C(17)–C(18)	1.397(14)
N(3)–Cu(1)	2.024(7)	C(19)–C(20)	1.380(10)
N(4)–C(3)	1.334(12)	C(19)–C(24)	1.437(11)
N(4)–C(9)	1.355(11)	C(20)–C(21)	1.436(11)
N(4)–Cu(1)	2.140(8)	C(21)–C(22)	1.361(12)
N(5)–C(4)	1.334(12)	C(22)–C(23)	1.470(10)
N(5)–C(10)	1.372(11)	C(23)–C(24)	1.407(11)
N(6)–C(5)	1.344(11)	C(25)–C(26)	1.431(14)
N(6)–C(11)	1.363(11)	C(27)–C(28)	1.407(14)
N(7)–C(13)	1.326(12)	C(29)–C(30)	1.393(13)
N(7)–C(19)	1.353(11)	C(31)–C(32)	1.402(12)
N(8)–C(18)	1.342(13)	C(31)–C(36)	1.456(11)
N(8)–C(24)	1.354(11)	C(32)–C(33)	1.439(11)
N(9)–C(17)	1.330(14)	C(33)–C(34)	1.419(11)
N(9)–C(23)	1.348(11)	C(34)–C(35)	1.438(11)
N(10)–C(16)	1.329(13)	C(35)–C(36)	1.407(12)
N(10)–C(22)	1.345(11)	C(1S)–C(2S)	1.3900
N(11)–C(15)	1.324(12)	C(1S)–C(6S)	1.3900
N(11)–C(21)	1.375(11)	C(2S)–C(3S)	1.3900
N(12)–C(14)	1.356(13)	C(3S)–C(4S)	1.3900
N(12)–C(20)	1.385(11)	C(4S)–C(5S)	1.3900
N(13)–C(25)	1.327(12)	C(5S)–C(6S)	1.3900
N(13)–C(31)	1.338(11)	C(7S)–C(8S)	1.3900
N(14)–C(30)	1.320(11)	C(7S)–C(12S)	1.3900
N(14)–C(36)	1.344(11)	C(8S)–C(9S)	1.3900
N(15)–C(29)	1.325(12)	C(9S)–C(10S)	1.3900
N(15)–C(35)	1.355(10)	C(10S)–C(11S)	1.3900
N(15)–Cu(4)	2.141(7)	C(11S)–C(12S)	1.3900
N(16)–C(28)	1.347(11)	C(13S)–C(14S)	1.3900
N(16)–C(34)	1.360(10)	C(13S)–C(18S)	1.3900
N(16)–Cu(4)	1.985(7)	C(14S)–C(15S)	1.3900
N(17)–C(33)	1.332(11)	C(15S)–C(16S)	1.3900
N(17)–C(27)	1.370(11)	C(16S)–C(17S)	1.3900

C(17S)–C(18S)	1.3900	N(2S)–O(4S)	1.192(15)
N(1S)–O(2S)	1.2513	N(2S)–O(3S)	1.298(16)
N(1S)–O(1S)	1.2534	N(2S)–C(20S)	1.459(16)
N(1S)–C(19S)	1.4804		

Table 3C. Bond angles (°) in the crystal structure of **3**.

F(6)–Sb(1)–F(1)	178.7(6)	F(16)–Sb(3)–F(14)	176.1(9)
F(6)–Sb(1)–F(2)	87.8(6)	F(18)–Sb(3)–F(14)	89.7(6)
F(1)–Sb(1)–F(2)	92.6(6)	F(17)–Sb(3)–F(13)	92.7(9)
F(6)–Sb(1)–F(3)	91.2(6)	F(15)–Sb(3)–F(13)	85.2(8)
F(1)–Sb(1)–F(3)	90.1(5)	F(16)–Sb(3)–F(13)	88.0(4)
F(2)–Sb(1)–F(3)	88.4(4)	F(18)–Sb(3)–F(13)	177.4(6)
F(6)–Sb(1)–F(4)	90.4(5)	F(14)–Sb(3)–F(13)	92.1(5)
F(1)–Sb(1)–F(4)	89.2(5)	F(20)–Sb(4)–F(19)	90.7(5)
F(2)–Sb(1)–F(4)	178.2(6)	F(20)–Sb(4)–F(22)	178.5(4)
F(3)–Sb(1)–F(4)	91.5(4)	F(19)–Sb(4)–F(22)	88.9(6)
F(6)–Sb(1)–F(5)	90.4(6)	F(20)–Sb(4)–F(21)	90.7(4)
F(1)–Sb(1)–F(5)	88.2(6)	F(19)–Sb(4)–F(21)	92.2(4)
F(2)–Sb(1)–F(5)	91.6(5)	F(22)–Sb(4)–F(21)	90.7(5)
F(3)–Sb(1)–F(5)	178.3(6)	F(20)–Sb(4)–F(24)	88.2(4)
F(4)–Sb(1)–F(5)	88.5(5)	F(19)–Sb(4)–F(24)	177.3(5)
F(9)–Sb(2)–F(7)	90.5(4)	F(22)–Sb(4)–F(24)	92.1(5)
F(9)–Sb(2)–F(12)	92.3(5)	F(21)–Sb(4)–F(24)	90.3(3)
F(7)–Sb(2)–F(12)	175.6(4)	F(20)–Sb(4)–F(23)	89.6(4)
F(9)–Sb(2)–F(10)	90.0(4)	F(19)–Sb(4)–F(23)	88.3(4)
F(7)–Sb(2)–F(10)	91.8(3)	F(22)–Sb(4)–F(23)	89.0(4)
F(12)–Sb(2)–F(10)	91.6(4)	F(21)–Sb(4)–F(23)	179.4(4)
F(9)–Sb(2)–F(8)	88.6(4)	F(24)–Sb(4)–F(23)	89.2(3)
F(7)–Sb(2)–F(8)	90.2(3)	N(2)–Cu(1)–N(3)	150.5(3)
F(12)–Sb(2)–F(8)	86.5(3)	N(2)–Cu(1)–N(4)	117.3(3))
F(10)–Sb(2)–F(8)	177.6(4)	N(3)–Cu(1)–N(4)	81.9(3))
F(9)–Sb(2)–F(11)	177.8(5)	N(2)–Cu(1)–N(1)	81.8(3)
F(7)–Sb(2)–F(11)	87.7(3)	N(3)–Cu(1)–N(1)	118.1(3)
F(12)–Sb(2)–F(11)	89.4(4)	N(4)–Cu(1)–N(1)	101.3(3)
F(10)–Sb(2)–F(11)	91.3(3)	N(8)–Cu(2)–N(6)	125.7(3)
F(8)–Sb(2)–F(11)	90.2(3)	N(8)–Cu(2)–N(5)	129.2(3)
F(17)–Sb(3)–F(15)	176.2(11)	N(6)–Cu(2)–N(5)	83.4(3)
F(17)–Sb(3)–F(16)	98.0(9)	N(8)–Cu(2)–N(7)	83.3(3)
F(15)–Sb(3)–F(16)	85.1(7)	N(6)–Cu(2)–N(7)	125.1(3)
F(17)–Sb(3)–F(18)	89.3(8)	N(5)–Cu(2)–N(7)	115.2(3)
F(15)–Sb(3)–F(18)	92.9(7)	N(12)–Cu(3)–N(14)	124.4(3)
F(16)–Sb(3)–F(18)	90.1(5)	N(12)–Cu(3)–N(11)	83.3(3)
F(17)–Sb(3)–F(14)	85.9(10)	N(14)–Cu(3)–N(11)	133.3(3)
F(15)–Sb(3)–F(14)	91.1(9)	N(12)–Cu(3)–N(13)	114.1(3)

N(14)–Cu(3)–N(13)	83.5(3)	C(29)–N(15)–C(35)	115.6(7)
N(11)–Cu(3)–N(13)	121.8(3)	C(29)–N(15)–Cu(4)	136.0(6)
N(16)–Cu(4)–N(17)	151.0(3)	C(35)–N(15)–Cu(4)	107.2(6)
N(16)–Cu(4)–N(18)	115.3(3)	C(28)–N(16)–C(34)	114.6(7)
N(17)–Cu(4)–N(18)	82.1(3)	C(28)–N(16)–Cu(4)	132.6(6)
N(16)–Cu(4)–N(15)	82.3(3)	C(34)–N(16)–Cu(4)	112.5(5)
N(17)–Cu(4)–N(15)	118.8(3)	C(33)–N(17)–C(27)	116.2(7)
N(18)–Cu(4)–N(15)	100.6(3)	C(33)–N(17)–Cu(4)	111.7(6)
C(12)–N(1)–C(6)	117.2(8)	C(27)–N(17)–Cu(4)	131.6(7)
C(12)–N(1)–Cu(1)	108.2(5)	C(26)–N(18)–C(32)	117.0(8)
C(6)–N(1)–Cu(1)	134.1(6)	C(26)–N(18)–Cu(4)	134.9(6)
C(1)–N(2)–C(7)	115.0(7)	C(32)–N(18)–Cu(4)	107.2(6)
C(1)–N(2)–Cu(1)	132.2(7)	N(2)–C(1)–C(2)	122.2(9)
C(7)–N(2)–Cu(1)	112.2(5)	N(3)–C(2)–C(1)	122.5(9)
C(2)–N(3)–C(8)	116.6(7)	N(4)–C(3)–C(4)	123.4(9)
C(2)–N(3)–Cu(1)	131.6(6)	N(5)–C(4)–C(3)	122.2(9)
C(8)–N(3)–Cu(1)	111.1(5))	N(6)–C(5)–C(6)	123.7(8)
C(3)–N(4)–C(9)	114.4(8)	N(1)–C(6)–C(5)	121.2(8)
C(3)–N(4)–Cu(1)	135.8(6)	N(2)–C(7)–C(8)	122.9(8)
C(9)–N(4)–Cu(1)	109.2(5)	N(2)–C(7)–C(12)	116.9(7)
C(4)–N(5)–C(10)	115.0(8)	C(8)–C(7)–C(12)	120.2(7)
C(4)–N(5)–Cu(2)	134.3(6)	N(3)–C(8)–C(7)	120.5(7)
C(10)–N(5)–Cu(2)	110.4(6)	N(3)–C(8)–C(9)	119.9(7)
C(5)–N(6)–C(11)	113.5(7)	C(7)–C(8)–C(9)	119.6(7)
C(5)–N(6)–Cu(2)	135.1(6)	N(4)–C(9)–C(10)	123.2(8)
C(11)–N(6)–Cu(2)	111.2(5)	N(4)–C(9)–C(8)	116.4(7)
C(13)–N(7)–C(19)	117.6(7)	C(10)–C(9)–C(8)	120.4(8)
C(13)–N(7)–Cu(2)	132.8(6)	C(9)–C(10)–N(5)	121.9(8)
C(19)–N(7)–Cu(2)	109.4(6)	C(9)–C(10)–C(11)	121.0(8)
C(18)–N(8)–C(24)	115.4(8)	N(5)–C(10)–C(11)	117.0(8)
C(18)–N(8)–Cu(2)	133.0(7)	N(6)–C(11)–C(12)	122.0(7)
C(24)–N(8)–Cu(2)	111.4(5)	N(6)–C(11)–C(10)	117.9(7)
C(17)–N(9)–C(23)	116.4(8)	C(12)–C(11)–C(10)	120.1(7)
C(16)–N(10)–C(22)	115.7(8)	N(1)–C(12)–C(11)	122.4(8)
C(15)–N(11)–C(21)	116.5(8)	N(1)–C(12)–C(7)	119.0(7)
C(15)–N(11)–Cu(3)	131.8(7)	C(11)–C(12)–C(7)	118.6(7)
C(21)–N(11)–Cu(3)	111.6(6)	N(7)–C(13)–C(14)	121.7(9)
C(14)–N(12)–C(20)	114.0(8)	N(12)–C(14)–C(13)	122.7(9)
C(14)–N(12)–Cu(3)	135.2(6)	N(11)–C(15)–C(16)	120.9(11)
C(20)–N(12)–Cu(3)	110.8(5)	N(10)–C(16)–C(15)	122.8(10)
C(25)–N(13)–C(31)	117.2(8)	N(9)–C(17)–C(18)	123.1(9)
C(25)–N(13)–Cu(3)	133.4(7)	N(8)–C(18)–C(17)	121.7(9)
C(31)–N(13)–Cu(3)	109.3(5)	N(7)–C(19)–C(20)	120.9(8)
C(30)–N(14)–C(36)	115.4(7)	N(7)–C(19)–C(24)	118.5(7)
C(30)–N(14)–Cu(3)	134.0(6)	C(20)–C(19)–C(24)	120.6(8)
C(36)–N(14)–Cu(3)	110.6(5)	C(19)–C(20)–N(12)	123.0(8)

C(19)–C(20)–C(21)	119.0(8)	C(33)–C(34)–C(35)	120.7(7)
N(12)–C(20)–C(21)	118.0(7)	N(15)–C(35)–C(36)	121.0(7)
C(22)–C(21)–N(11)	121.1(7)	N(15)–C(35)–C(34)	118.8(7)
C(22)–C(21)–C(20)	122.5(7)	C(36)–C(35)–C(34)	120.2(7)
N(11)–C(21)–C(20)	116.4(7)	N(14)–C(36)–C(35)	122.4(7)
N(10)–C(22)–C(21)	122.8(8)	N(14)–C(36)–C(31)	118.1(7)
N(10)–C(22)–C(23)	118.3(7)	C(35)–C(36)–C(31)	119.4(7)
C(21)–C(22)–C(23)	118.9(7)	C(2S)–C(1S)–C(6S)	120.0
N(9)–C(23)–C(24)	120.7(8)	C(3S)–C(2S)–C(1S)	120.0
N(9)–C(23)–C(22)	120.5(8)	C(2S)–C(3S)–C(4S)	120.0
C(24)–C(23)–C(22)	118.8(7)	C(5S)–C(4S)–C(3S)	120.0
N(8)–C(24)–C(23)	122.8(7)	C(6S)–C(5S)–C(4S)	120.0
N(8)–C(24)–C(19)	117.2(7)	C(5S)–C(6S)–C(1S)	120.0
C(23)–C(24)–C(19)	120.1(7)	C(8S)–C(7S)–C(12S)	120.0
N(13)–C(25)–C(26)	120.4(9)	C(9S)–C(8S)–C(7S)	120.0
N(18)–C(26)–C(25)	122.6(8)	C(8S)–C(9S)–C(10S)	120.0
N(17)–C(27)–C(28)	120.6(8)	C(11S)–C(10S)–C(9S)	120.0
N(16)–C(28)–C(27)	123.7(8)	C(12S)–C(11S)–C(10S)	120.0
N(15)–C(29)–C(30)	122.7(8)	C(11S)–C(12S)–C(7S)	120.0
N(14)–C(30)–C(29)	122.9(8)	C(14S)–C(13S)–C(18S)	120.0
N(13)–C(31)–C(32)	121.7(7)	C(15S)–C(14S)–C(13S)	120.0
N(13)–C(31)–C(36)	118.4(7)	C(14S)–C(15S)–C(16S)	120.0
C(32)–C(31)–C(36)	119.8(7)	C(15S)–C(16S)–C(17S)	120.0
N(18)–C(32)–C(31)	121.1(7)	C(18S)–C(17S)–C(16S)	120.0
N(18)–C(32)–C(33)	117.7(7)	C(17S)–C(18S)–C(13S)	120.0
C(31)–C(32)–C(33)	121.2(7)	O(2S)–N(1S)–O(1S)	122.0
N(17)–C(33)–C(34)	122.5(7)	O(2S)–N(1S)–C(19S)	115.9
N(17)–C(33)–C(32)	118.9(7)	O(1S)–N(1S)–C(19S)	122.1
C(34)–C(33)–C(32)	118.6(7)	O(4S)–N(2S)–O(3S)	124(2)
N(16)–C(34)–C(33)	121.9(7)	O(4S)–N(2S)–C(20S)	123(2)
N(16)–C(34)–C(35)	117.4(7)	O(3S)–N(2S)–C(20S)	113.0(18)