Supporting Information

Complex 1

- Figure F1 : Ortep plot of the cationic part of 1 with the labelling scheme used (partial). Ellipsoids are scaled to enclose 30% of the electronic density. Hydrogen atoms are omitted.
- Table S1 : crystallographic data (1 page)
- Table S2 : atomic coordinates and thermal equivalent parameters for non hydrogen atoms (6 pages)
- Table S3 : atomic coordinates and thermal equivalent parameters for hydrogen atoms (4 pages)
- Table S4 : thermal parameters for anisotropic atoms (6 pages)
- Table S5 : bond distances (Å) (3 pages)
- Table S6 : bond angles (deg) (5 pages)

Complex 2

- Figure F2 : Ortep plot of the cationic part of 1 with the labelling scheme used (partial). Ellipsoids are scaled to enclose 30% of the electronic density. Hydrogen atoms are omitted.
- Table S7 : crystallographic data (1 page)
- Table S8 : atomic coordinates and thermal equivalent parameters for non hydrogen atoms (7 pages)
- Table S9 : atomic coordinates and thermal equivalent parameters for hydrogen atoms (4 pages)
- Table S10 : thermal parameters for anisotropic atoms (6 pages)
- Table S11 : bond distances (Å) (4 pages)
- Table S12 : bond angles (deg) (7 pages)

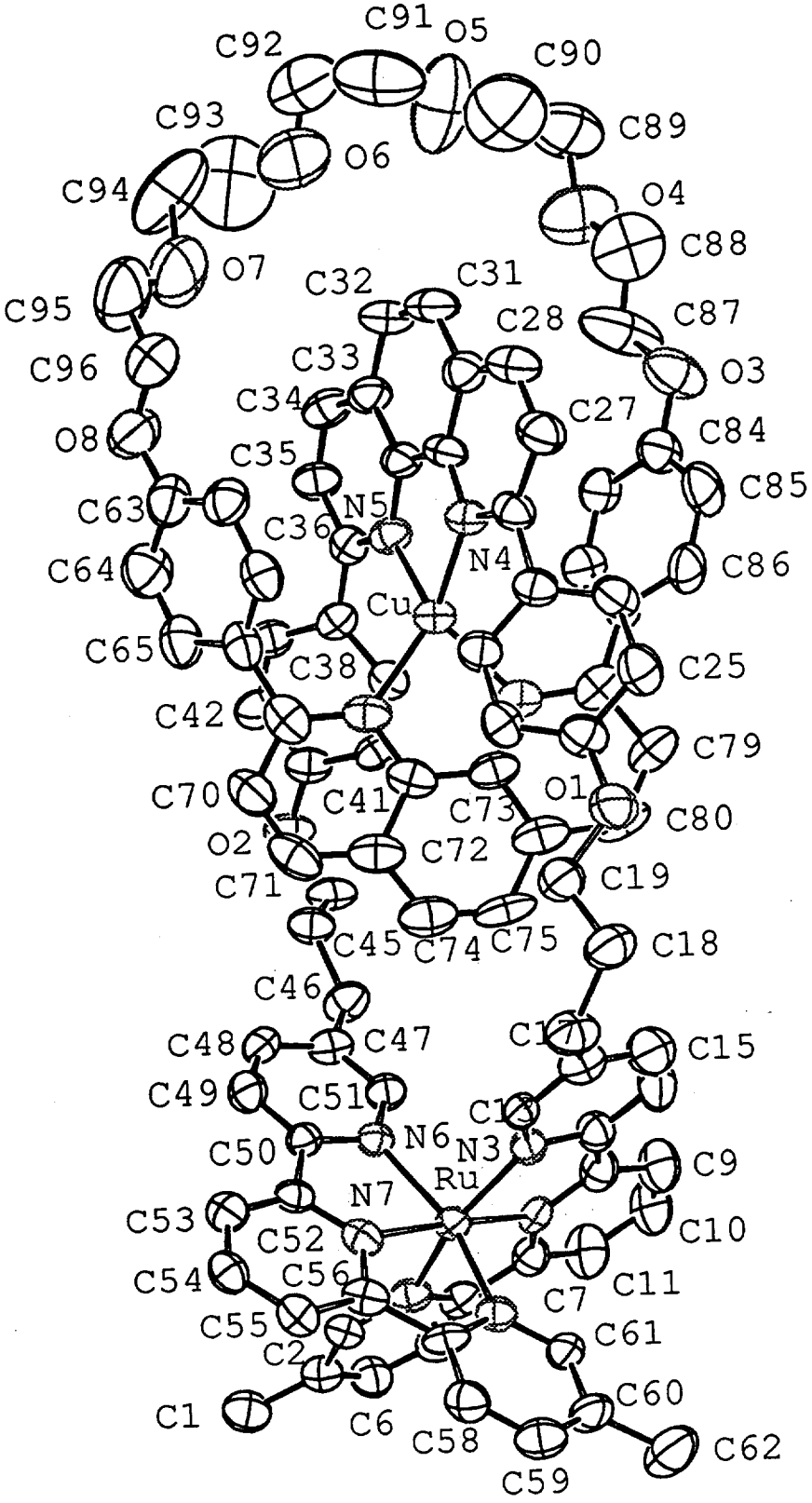
C91
O5
C92
C90
C93
C89
O6
C94
O4
C88
O7
C32
C31
C95
C28
C87
C96
C33
O3
C34
C27
O8
C84
C35
C85
C63
N5
C36
N4
C64
C86
Cu
C65
C38
C25
C42
C79
C70
C41
C73
O1
C80
O2
C72
C71
C19
C45
C74
C75
C18
C46
C48
C47
C15
C49
C51
C50
N6
N3
C9
N7
Ru
C53
C10
C52
C54
C56
C7
C11
C55
C61
C2
C60
C1
C6
C58
C62
C59

Table 1 : X-ray experimental data

Formula	: $C_{103}H_{104}N_{12}O_{12}F_{18}P_3CuRu$
Molecular weight	: 2301.55
Crystal system	: triclinic
Space group	: P-1
a(Å)	: 17.174(5)
b(Å)	: 24.252(7)
c(Å)	: 13.223(4)
α(deg)	: 92.90(2)
β(deg)	: 95.00(2)
γ(deg)	: 91.86(2)
V(Å^3)	: 5475(5)
Z	: 2
Color	: dark red
Crystal dim(mm)	: 0.40*0.40*0.30
Dcalc(gcm^{-3})	: 1.40
F000	: 2364
μ(mm^{-1})	: 2.594
Trans. min and max	: 0.53/1.00
Temperature(K)	: 173
Wavelength(Å)	: 1.54184
Radiation	: CuKα graphite monochromated
Diffractometer	: Philips_PW1100
Scan mode	: θ/2θ
hkl limits	: -18,17/-25,25/0,13
Theta limits(deg)	: 3.0/54.07
Number of data meas.	: 13282
Number of data with I > 3 σ(I)	: 8946
Weighting scheme	: $4Fo^2/(\sigma^2(Fo2)+0.0025\ Fo^4)+5.0$
Number of variables	: 1301
R	: 0.084
Rw	: 0.121
GOF	: 1.533
Largest peak in final difference (eÅ^{-3})	: 2.382

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
RU	0.73374(5)	0.05763(3)	0.35244(6)	0.0353(4)
CU	0.76369(9)	0.48555(6)	0.4660(1)	0.0441(9)
C1	0.5787(7)	-0.0882(5)	0.588(1)	0.062(8)
C2	0.5765(7)	-0.0576(4)	0.4913(9)	0.048(6)
C3	0.6418(6)	-0.0246(4)	0.4709(8)	0.043(6)
N1	0.6446(5)	0.0044(3)	0.3896(7)	0.041(5)
C4	0.5806(6)	0.0030(5)	0.3193(9)	0.046(6)
C5	0.5146(6)	-0.0299(5)	0.336(1)	0.052(7)
C6	0.5138(7)	-0.0593(5)	0.4218(9)	0.052(7)
C7	0.5865(7)	0.0379(5)	0.2329(8)	0.047(6)
N2	0.6553(5)	0.0674(3)	0.2385(6)	0.035(4)
C8	0.6718(6)	0.1023(5)	0.1648(9)	0.048(6)
C9	0.6183(8)	0.1083(6)	0.082(1)	0.064(8)
C10	0.5482(8)	0.0791(6)	0.077(1)	0.068(8)
C11	0.5303(7)	0.0435(6)	0.153(1)	0.063(8)
C12	0.7506(6)	0.1276(5)	0.1834(8)	0.046(6)
N3	0.7914(5)	0.1136(3)	0.2703(6)	0.037(4)
C13	0.8643(6)	0.1356(4)	0.2901(8)	0.041(6)
C14	0.9026(7)	0.1688(5)	0.2260(9)	0.052(7)
C15	0.8593(8)	0.1815(6)	0.138(1)	0.070(8)
C16	0.7828(8)	0.1613(6)	0.1170(9)	0.059(7)
C17	0.9881(7)	0.1858(5)	0.251(1)	0.062(7)
C18	1.0135(8)	0.2431(5)	0.219(1)	0.064(8)
C19	0.9819(7)	0.2889(5)	0.284(1)	0.060(7)
O1	0.9938(5)	0.3392(3)	0.2320(6)	0.067(5)
C20	0.9712(7)	0.3875(5)	0.276(1)	0.053(7)
C21	0.9510(6)	0.3942(5)	0.3748(9)	0.051(6)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C22	0.9303(6)	0.4452(4)	0.4118(9)	0.047(6)
C23	0.9305(6)	0.4907(5)	0.3509(9)	0.049(6)
C24	0.9525(7)	0.4842(5)	0.2541(9)	0.056(7)
C25	0.9734(7)	0.4336(5)	0.216(1)	0.063(8)
C26	0.9063(6)	0.5452(5)	0.3878(9)	0.047(6)
C27	0.9468(7)	0.5948(5)	0.367(1)	0.060(7)
C28	0.9258(8)	0.6440(5)	0.409(1)	0.060(8)
C29	0.8623(7)	0.6471(5)	0.4682(9)	0.053(7)
C30	0.8191(7)	0.5964(4)	0.4796(9)	0.046(6)
N4	0.8421(5)	0.5470(3)	0.4429(7)	0.043(5)
C31	0.8376(8)	0.6961(5)	0.517(1)	0.059(8)
C32	0.7754(8)	0.6960(5)	0.572(1)	0.060(8)
C33	0.7311(7)	0.6470(5)	0.5818(9)	0.052(7)
C34	0.6640(7)	0.6450(5)	0.635(1)	0.057(7)
C35	0.6225(7)	0.5966(5)	0.637(1)	0.056(7)
C36	0.6441(6)	0.5480(4)	0.5848(8)	0.045(6)
N5	0.7074(5)	0.5487(3)	0.5333(7)	0.044(5)
C37	0.7513(7)	0.5975(4)	0.5319(9)	0.047(6)
C38	0.5981(6)	0.4964(4)	0.5890(8)	0.044(6)
C39	0.5924(6)	0.4555(5)	0.5106(8)	0.045(6)
C40	0.5527(6)	0.4055(4)	0.5168(8)	0.043(6)
C41	0.5158(6)	0.3957(4)	0.6032(9)	0.046(6)
C42	0.5198(7)	0.4359(5)	0.683(1)	0.056(7)
C43	0.5588(7)	0.4848(5)	0.6740(9)	0.051(7)
O2	0.4728(4)	0.3498(3)	0.6197(7)	0.060(5)
C44	0.4769(7)	0.3019(5)	0.551(1)	0.054(7)
C45	0.5514(7)	0.2721(5)	0.575(1)	0.054(7)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C46	0.5485(7)	0.2167(5)	0.516(1)	0.057(7)
C47	0.6183(6)	0.1809(4)	0.5321(9)	0.047(6)
C48	0.6599(7)	0.1778(5)	0.6249(9)	0.047(6)
C49	0.7205(7)	0.1416(5)	0.6358(9)	0.049(6)
C50	0.7408(6)	0.1099(4)	0.5555(8)	0.037(6)
N6	0.6999(5)	0.1141(3)	0.4616(6)	0.037(4)
C51	0.6425(6)	0.1496(4)	0.4527(8)	0.042(6)
C52	0.8022(6)	0.0699(4)	0.5599(8)	0.039(6)
C53	0.8487(6)	0.0557(5)	0.6436(9)	0.045(6)
C54	0.9023(6)	0.0142(5)	0.6326(9)	0.048(6)
C55	0.9085(6)	-0.0125(4)	0.5403(8)	0.043(6)
C56	0.8610(6)	0.0028(4)	0.4572(9)	0.038(6)
N7	0.8096(5)	0.0438(3)	0.4679(7)	0.039(5)
C57	0.8550(6)	-0.0228(4)	0.3521(9)	0.040(6)
C58	0.9030(7)	-0.0637(5)	0.3214(9)	0.050(7)
C59	0.8904(7)	-0.0864(5)	0.224(1)	0.062(7)
C60	0.8319(7)	-0.0686(5)	0.1578(9)	0.054(7)
C61	0.7860(7)	-0.0275(4)	0.1939(8)	0.046(6)
N8	0.7961(5)	-0.0040(3)	0.2885(6)	0.038(5)
C62	0.816(1)	-0.0926(6)	0.050(1)	0.083(9)
C63	0.7819(8)	0.5560(6)	0.822(1)	0.067(8)
C64	0.7346(9)	0.5105(7)	0.842(1)	0.08(1)
C65	0.7355(8)	0.4610(6)	0.788(1)	0.067(8)
C66	0.7838(7)	0.4555(5)	0.7089(9)	0.056(7)
C67	0.8330(7)	0.5002(5)	0.6921(9)	0.057(7)
C68	0.8333(7)	0.5502(5)	0.7488(9)	0.059(7)
C69	0.7790(7)	0.4061(5)	0.639(1)	0.056(7)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C70	0.7813(8)	0.3530(5)	0.676(1)	0.068(8)
C71	0.7800(7)	0.3094(5)	0.610(1)	0.070(8)
C72	0.7710(7)	0.3147(5)	0.504(1)	0.056(7)
C73	0.7659(6)	0.3698(5)	0.471(1)	0.049(6)
N9	0.7720(5)	0.4137(4)	0.5379(7)	0.046(5)
C74	0.7672(7)	0.2711(5)	0.426(1)	0.065(8)
C75	0.7598(8)	0.2798(5)	0.329(1)	0.066(8)
C76	0.7515(7)	0.3349(5)	0.295(1)	0.061(8)
C77	0.7531(6)	0.3790(5)	0.366(1)	0.048(6)
N10	0.7435(5)	0.4325(4)	0.3417(7)	0.045(5)
C78	0.7365(7)	0.4439(5)	0.2420(9)	0.054(7)
C79	0.7390(8)	0.4011(6)	0.164(1)	0.067(8)
C80	0.7464(8)	0.3482(5)	0.193(1)	0.069(8)
C81	0.7288(7)	0.5034(5)	0.2204(8)	0.049(7)
C82	0.6825(7)	0.5362(5)	0.2731(9)	0.054(7)
C83	0.6796(7)	0.5918(5)	0.2639(9)	0.054(7)
C84	0.7272(7)	0.6164(5)	0.197(1)	0.063(7)
C85	0.7725(8)	0.5841(6)	0.140(1)	0.072(8)
C86	0.7743(7)	0.5275(5)	0.1504(9)	0.061(7)
O3	0.7326(6)	0.6722(4)	0.1889(8)	0.095(6)
C87	0.692(1)	0.7073(7)	0.258(2)	0.12(1)
C88	0.723(1)	0.7636(9)	0.266(2)	0.13(2)
O4	0.6765(7)	0.7934(5)	0.331(1)	0.122(9)
C89	0.714(1)	0.8474(7)	0.363(2)	0.12(1)
C90	0.767(2)	0.848(1)	0.448(2)	0.17(2)
O5	0.7472(8)	0.8546(7)	0.532(1)	0.15(1)
C91	0.809(1)	0.8586(7)	0.616(2)	0.11(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
F17	0.2904(9)	0.6658(6)	0.078(2)	0.159(4)	*
F18	0.360(1)	0.7295(7)	-0.005(1)	0.241(4)	*
N11	0.385(1)	0.108(2)	0.873(2)	0.16(1)	
C97	0.434(1)	0.139(1)	0.846(2)	0.17(2)	
C98	0.491(1)	0.167(1)	0.801(2)	0.15(2)	
N12	0.023(2)	0.192(1)	0.961(3)	0.08(2)	
C99	0.048(2)	0.228(1)	0.913(3)	0.09(2)	
C100	0.079(2)	0.280(2)	0.852(2)	0.11(2)	
O9	0.459(2)	0.752(1)	0.788(3)	0.13(2)	
C101	0.467(2)	0.696(1)	0.738(3)	0.13(2)	
O10	-0.014(2)	0.583(1)	0.060(3)	0.16(1)	
C102	0.082(2)	0.577(2)	0.058(3)	0.13(3)	
O11	0.924(1)	0.0664(9)	0.978(2)	0.16(1)	
O12	0.0392(9)	0.9490(6)	0.908(1)	0.16(1)	
C103	0.016(1)	0.9579(8)	0.831(1)	0.14(1)	

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor. Starred atoms were refined isotropically.

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
C92	0.774(1)	0.8585(9)	0.714(2)	0.13(2)	
O6	0.731(1)	0.8131(5)	0.716(1)	0.15(1)	
C93	0.679(2)	0.805(2)	0.802(3)	0.167(8)	*
C94	0.729(2)	0.7850(9)	0.874(2)	0.17(2)	
O7	0.745(1)	0.7263(6)	0.846(1)	0.14(1)	
C95	0.791(1)	0.7014(9)	0.909(1)	0.12(1)	
C96	0.821(1)	0.6504(7)	0.863(1)	0.09(1)	
O8	0.7720(6)	0.6049(4)	0.8783(7)	0.085(6)	
P1	0.7041(2)	0.0226(1)	0.8515(3)	0.057(2)	
F1	0.7209(4)	0.0224(3)	0.9715(5)	0.074(5)	
F2	0.6235(4)	0.0524(3)	0.8651(6)	0.072(5)	
F3	0.7493(4)	0.0811(3)	0.8516(6)	0.072(4)	
F4	0.7839(4)	-0.0076(3)	0.8365(6)	0.077(5)	
F5	0.6582(4)	-0.0356(3)	0.8498(7)	0.082(5)	
F6	0.6867(4)	0.0232(3)	0.7302(5)	0.071(5)	
P2	0.9698(2)	0.1945(1)	0.5859(3)	0.053(2)	
F7	0.9627(5)	0.1580(3)	0.6804(6)	0.084(5)	
F8	0.9523(5)	0.2485(3)	0.6509(7)	0.081(5)	
F9	1.0594(4)	0.2044(4)	0.6198(8)	0.088(6)	
F10	0.9872(5)	0.1400(3)	0.5207(6)	0.082(5)	
F11	0.8803(4)	0.1838(3)	0.5529(8)	0.086(6)	
F12	0.9796(6)	0.2308(3)	0.4914(6)	0.099(6)	
P3	0.3147(4)	0.7298(3)	0.0882(5)	0.150(4)	*
F13	0.260(1)	0.7363(6)	0.180(1)	0.232(4)	*
F14	0.3857(9)	0.7216(6)	0.160(1)	0.241(4)	*
F15	0.3267(9)	0.7961(7)	0.101(2)	0.154(4)	*
F16	0.237(1)	0.7383(6)	0.017(1)	0.164(4)	*

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	0.5307	-0.1084	0.5902	0.0808	*
H2	0.6205	-0.1130	0.5893	0.0808	*
H3	0.5865	-0.0626	0.6447	0.0808	*
H4	0.6865	-0.0232	0.5187	0.0563	*
H5	0.4704	-0.0319	0.2873	0.0754	*
H6	0.4685	-0.0811	0.4325	0.0685	*
H7	0.6299	0.1320	0.0298	0.0867	*
H8	0.5110	0.0829	0.0202	0.0945	*
H9	0.4811	0.0241	0.1501	0.0876	*
H10	0.7529	0.1708	0.0570	0.0802	*
H11	0.8821	0.2043	0.0909	0.0901	*
H12	0.8919	0.1279	0.3529	0.0545	*
H13	1.0182	0.1595	0.2172	0.0808	*
H14	0.9995	0.1848	0.3220	0.0808	*
H15	0.9950	0.2469	0.1504	0.0838	*
H16	1.0690	0.2463	0.2265	0.0838	*
H17	1.0093	0.2917	0.3495	0.0778	*
H18	0.9277	0.2821	0.2898	0.0778	*
H19	0.9515	0.3637	0.4171	0.0652	*
H20	0.9156	0.4495	0.4793	0.0612	*
H21	0.9534	0.5152	0.2129	0.0718	*
H22	0.9892	0.4297	0.1485	0.0814	*
H23	0.9884	0.5936	0.3240	0.0779	*
H24	0.9548	0.6768	0.3974	0.0825	*
H25	0.8658	0.7299	0.5107	0.0844	*
H26	0.7613	0.7295	0.6055	0.0841	*
H27	0.6476	0.6774	0.6686	0.0754	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H28	0.5779	0.5953	0.6745	0.0749	*
H29	0.6167	0.4624	0.4504	0.0588	*
H30	0.5509	0.3782	0.4623	0.0565	*
H31	0.4954	0.4291	0.7427	0.0724	*
H32	0.5594	0.5123	0.7280	0.0662	*
H33	0.4753	0.3133	0.4833	0.0747	*
H34	0.4334	0.2775	0.5575	0.0747	*
H35	0.5576	0.2664	0.6461	0.0712	*
H36	0.5945	0.2939	0.5574	0.0712	*
H37	0.5420	0.2237	0.4460	0.0756	*
H38	0.5042	0.1962	0.5341	0.0756	*
H39	0.6472	0.2004	0.6815	0.0630	*
H40	0.7482	0.1390	0.7007	0.0651	*
H41	0.6168	0.1535	0.3870	0.0543	*
H42	0.8446	0.0739	0.7081	0.0596	*
H43	0.9349	0.0043	0.6902	0.0627	*
H44	0.9446	-0.0410	0.5332	0.0564	*
H45	0.9439	-0.0761	0.3668	0.0659	*
H46	0.9228	-0.1148	0.2018	0.0828	*
H47	0.7448	-0.0151	0.1491	0.0598	*
H48	0.8523	-0.1202	0.0377	0.1121	*
H49	0.7643	-0.1087	0.0413	0.1121	*
H50	0.8205	-0.0642	0.0041	0.1121	*
H51	0.7007	0.5140	0.8948	0.1077	*
H52	0.7033	0.4306	0.8037	0.0874	*
H53	0.8676	0.4964	0.6401	0.0750	*
H54	0.8684	0.5798	0.7368	0.0784	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H55	0.7837	0.3481	0.7471	0.0889	*
H56	0.7854	0.2736	0.6353	0.0927	*
H57	0.7702	0.2341	0.4463	0.0925	*
H58	0.7600	0.2495	0.2807	0.0919	*
H59	0.7357	0.4093	0.0947	0.0888	*
H60	0.7481	0.3193	0.1419	0.0940	*
H61	0.6504	0.5196	0.3190	0.0699	*
H62	0.6460	0.6134	0.3019	0.0703	*
H63	0.8033	0.6007	0.0928	0.0919	*
H64	0.8060	0.5055	0.1104	0.0800	*
H65	0.6977	0.6928	0.3236	0.1740	*
H66	0.6384	0.7070	0.2342	0.1740	*
H67	0.7191	0.7786	0.2006	0.1671	*
H68	0.7758	0.7651	0.2931	0.1671	*
H69	0.6736	0.8720	0.3780	0.1701	*
H70	0.7397	0.8603	0.3080	0.1701	*
H71	0.8054	0.8761	0.4401	0.2259	*
H72	0.7913	0.8128	0.4455	0.2259	*
H73	0.8396	0.8919	0.6133	0.1766	*
H74	0.8422	0.8280	0.6109	0.1766	*
H75	0.7421	0.8896	0.7204	0.1678	*
H76	0.8138	0.8600	0.7686	0.1678	*
H77	0.6375	0.7789	0.7820	0.3124	*
H78	0.6591	0.8386	0.8249	0.3124	*
H79	0.7073	0.7871	0.9373	0.2268	*
H80	0.7771	0.8064	0.8793	0.2268	*
H81	0.7624	0.6919	0.9650	0.1625	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H82	0.8335	0.7258	0.9330	0.1625	*
H83	0.8722	0.6447	0.8938	0.1250	*
H84	0.8233	0.6542	0.7922	0.1250	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
RU	.0337(4)	.0348(4)	.0373(4)	.0048(3)	-.0004(3)	.0002(3)
CU	.0471(9)	.0343(8)	.0530(9)	.0002(7)	.0038(8)	.0003(7)
C1	.061(7)	.053(7)	.073(8)	-.008(6)	.012(7)	.008(7)
C2	.050(6)	.040(6)	.057(7)	.001(5)	.008(6)	.003(6)
C3	.046(6)	.036(6)	.049(6)	.002(5)	.005(5)	.006(5)
N1	.037(5)	.035(5)	.051(5)	.004(4)	.001(4)	-.001(4)
C4	.045(6)	.044(6)	.051(7)	.004(5)	-.004(6)	-.008(5)
C5	.031(6)	.059(7)	.078(8)	-.007(6)	-.013(6)	-.014(7)
C6	.050(7)	.051(7)	.056(7)	-.011(6)	-.001(6)	.006(6)
C7	.047(6)	.051(6)	.042(6)	.008(5)	-.003(5)	.000(5)
N2	.034(4)	.043(5)	.029(4)	.010(4)	-.001(4)	-.005(4)
C8	.047(6)	.054(7)	.045(6)	.012(5)	-.004(5)	-.001(6)
C9	.059(7)	.090(9)	.049(7)	-.005(7)	-.010(6)	.010(7)
C10	.058(8)	.10(1)	.052(7)	.009(8)	-.017(6)	.011(8)
C11	.044(7)	.10(1)	.055(7)	-.007(7)	-.009(6)	.011(7)
C12	.049(6)	.048(6)	.042(6)	.008(5)	.005(5)	.002(5)
N3	.037(4)	.037(4)	.038(5)	.005(4)	.004(4)	-.000(4)
C13	.053(6)	.036(5)	.037(6)	.008(5)	.003(5)	-.002(5)
C14	.046(6)	.052(7)	.058(7)	.000(6)	.006(6)	-.004(6)
C15	.069(8)	.071(8)	.070(8)	-.007(7)	.022(7)	.002(7)
C16	.066(8)	.079(8)	.040(6)	-.004(7)	.003(6)	.011(6)
C17	.058(7)	.056(7)	.073(8)	-.008(6)	.018(6)	-.001(7)
C18	.069(8)	.055(7)	.070(8)	-.006(6)	.021(7)	-.010(7)
C19	.069(8)	.053(7)	.058(7)	-.006(6)	.016(6)	-.003(6)
O1	.086(5)	.052(5)	.068(5)	.003(4)	.032(4)	.005(4)
C20	.051(6)	.044(6)	.069(8)	.009(5)	.011(6)	.004(6)
C21	.044(6)	.058(7)	.051(7)	.001(6)	.014(5)	.010(6)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C22	.044(6)	.044(6)	.054(7)	-.001(5)	.007(5)	.005(6)
C23	.044(6)	.043(6)	.060(7)	-.007(5)	.005(6)	.003(6)
C24	.056(7)	.047(6)	.065(7)	.004(6)	.016(6)	.011(6)
C25	.064(7)	.070(8)	.057(7)	.004(7)	.016(6)	.013(7)
C26	.043(6)	.043(6)	.056(7)	-.004(5)	-.005(6)	.008(6)
C27	.060(7)	.055(7)	.065(8)	-.012(6)	.005(6)	.011(6)
C28	.066(8)	.037(6)	.086(9)	-.012(6)	.004(7)	.006(6)
C29	.060(7)	.045(6)	.056(7)	-.001(6)	-.007(6)	.004(6)
C30	.053(6)	.033(6)	.057(7)	-.005(5)	-.003(6)	.010(5)
N4	.043(5)	.034(5)	.052(5)	-.004(4)	.002(4)	.001(4)
C31	.071(8)	.032(6)	.088(9)	-.008(6)	-.005(8)	-.001(6)
C32	.069(8)	.036(6)	.087(9)	-.010(6)	.002(7)	-.003(7)
C33	.070(8)	.039(6)	.053(7)	.012(6)	-.005(6)	-.002(6)
C34	.056(7)	.046(6)	.070(8)	.011(6)	-.002(6)	-.010(6)
C35	.053(7)	.045(6)	.074(8)	.010(6)	.007(6)	-.006(6)
C36	.041(6)	.045(6)	.048(6)	.011(5)	-.003(5)	.003(5)
N5	.045(5)	.038(5)	.050(5)	.004(4)	-.005(4)	-.001(4)
C37	.053(6)	.042(6)	.046(6)	-.004(5)	-.009(6)	.003(5)
C38	.039(6)	.043(6)	.050(6)	.012(5)	.002(5)	-.005(5)
C39	.040(6)	.048(6)	.047(6)	.006(5)	.001(5)	.005(5)
C40	.038(6)	.043(6)	.049(6)	.003(5)	.006(5)	-.006(5)
C41	.036(6)	.039(6)	.070(8)	.008(5)	.007(6)	-.002(6)
C42	.046(6)	.053(7)	.070(8)	.003(6)	.021(6)	-.004(6)
C43	.047(6)	.045(6)	.060(7)	.008(5)	.006(6)	-.004(6)
O2	.060(4)	.039(4)	.093(6)	.006(4)	.036(4)	-.006(4)
C44	.046(6)	.039(6)	.088(9)	-.001(5)	.015(6)	-.003(6)
C45	.050(6)	.043(6)	.072(8)	.011(5)	.008(6)	.001(6)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C46	.051(7)	.054(7)	.067(8)	.018(6)	-.004(6)	-.009(6)
C47	.043(6)	.038(6)	.063(7)	-.000(5)	.007(6)	-.002(6)
C48	.056(7)	.042(6)	.046(6)	.000(5)	-.002(6)	-.005(5)
C49	.056(7)	.048(6)	.045(6)	.002(6)	-.005(6)	.005(6)
C50	.042(6)	.032(5)	.039(6)	-.001(5)	-.001(5)	-.001(5)
N6	.037(4)	.032(4)	.040(5)	.003(4)	.004(4)	-.001(4)
C51	.040(6)	.038(6)	.048(6)	.006(5)	.004(5)	.000(5)
C52	.039(5)	.032(5)	.046(6)	-.005(5)	.006(5)	.004(5)
C53	.040(6)	.045(6)	.051(6)	-.005(5)	-.004(5)	.005(5)
C54	.042(6)	.054(7)	.049(6)	.006(5)	-.006(5)	.015(5)
C55	.034(5)	.046(6)	.052(6)	.006(5)	.007(5)	.009(5)
C56	.023(5)	.039(6)	.061(7)	.001(5)	-.001(5)	.007(5)
N7	.034(4)	.035(4)	.049(5)	-.002(4)	-.005(4)	.008(4)
C57	.035(5)	.030(5)	.062(7)	.005(5)	.006(5)	-.009(5)
C58	.049(6)	.046(6)	.055(7)	.007(5)	-.009(6)	.003(6)
C59	.060(7)	.047(7)	.086(9)	.019(6)	.010(7)	.001(7)
C60	.065(7)	.046(6)	.053(7)	.018(6)	-.002(6)	-.007(6)
C61	.053(6)	.041(6)	.044(6)	.008(5)	.000(5)	-.001(5)
N8	.033(4)	.039(5)	.045(5)	.007(4)	.002(4)	.002(4)
C62	.11(1)	.076(9)	.069(9)	.034(8)	-.015(9)	-.022(8)
C63	.065(8)	.083(9)	.055(8)	-.007(7)	.001(7)	-.001(7)
C64	.077(9)	.09(1)	.078(9)	-.006(8)	.016(8)	.009(9)
C65	.063(8)	.083(9)	.057(8)	-.006(7)	.010(6)	.008(7)
C66	.054(7)	.068(8)	.048(7)	.001(6)	.003(6)	.012(6)
C67	.046(6)	.071(8)	.058(7)	.003(6)	.005(6)	.018(6)
C68	.055(7)	.069(8)	.055(7)	-.009(6)	-.000(6)	-.002(7)
C69	.039(6)	.064(7)	.073(8)	.004(6)	.001(6)	.023(6)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C70	.074(8)	.057(7)	.075(9)	.001(7)	-.001(7)	.018(7)
C71	.054(7)	.065(7)	.097(9)	.010(6)	.000(7)	.037(7)
C72	.036(6)	.050(7)	.097(9)	.001(6)	.005(6)	.001(7)
C73	.035(6)	.043(6)	.078(8)	.006(5)	.004(6)	.012(6)
N9	.037(5)	.039(5)	.068(6)	-.000(4)	-.001(5)	.002(5)
C74	.051(7)	.048(7)	.11(1)	-.004(6)	.008(8)	-.008(8)
C75	.065(8)	.043(6)	.10(1)	.011(6)	.006(7)	-.029(7)
C76	.053(7)	.048(7)	.090(9)	.005(6)	.006(7)	-.015(7)
C77	.036(6)	.042(6)	.074(8)	-.003(5)	.006(6)	-.010(6)
N10	.037(5)	.040(5)	.061(6)	.004(4)	.008(4)	-.000(5)
C78	.040(6)	.064(7)	.061(7)	.008(6)	.004(6)	-.012(6)
C79	.074(8)	.070(8)	.058(8)	.006(7)	.003(7)	-.024(7)
C80	.080(9)	.051(7)	.080(9)	-.000(7)	.001(8)	-.035(7)
C81	.056(7)	.059(7)	.036(6)	.011(6)	.002(5)	.003(6)
C82	.047(6)	.056(7)	.059(7)	.004(6)	.011(6)	.002(6)
C83	.048(6)	.060(7)	.055(7)	.007(6)	.011(6)	-.002(6)
C84	.064(7)	.058(7)	.066(8)	.003(6)	.022(6)	.010(6)
C85	.079(8)	.083(9)	.056(7)	.012(7)	.034(6)	.017(7)
C86	.073(8)	.071(8)	.044(6)	.016(7)	.022(6)	.000(6)
O3	.097(6)	.067(6)	.133(7)	.015(5)	.064(5)	.023(6)
C87	.12(1)	.057(9)	.24(2)	.018(8)	.10(1)	.03(1)
C88	.11(1)	.13(2)	.15(2)	.00(1)	.03(1)	.01(1)
O4	.106(8)	.091(7)	.19(1)	.031(6)	.036(8)	-.025(8)
C89	.16(2)	.07(1)	.17(2)	.02(1)	.04(1)	.01(1)
C90	.18(2)	.17(2)	.18(2)	.06(2)	-.01(2)	.00(2)
O5	.145(9)	.22(1)	.111(9)	.101(8)	.018(8)	-.015(9)
C91	.08(1)	.08(1)	.25(2)	.016(9)	-.03(1)	.03(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C92	.13(2)	.11(1)	.14(2)	.00(1)	-.01(1)	-.03(1)
O6	.23(2)	.083(8)	.16(1)	.030(9)	.04(1)	-.025(8)
C94	.20(2)	.18(2)	.13(1)	.07(1)	.02(1)	-.10(1)
O7	.25(2)	.123(9)	.093(9)	.06(1)	.01(1)	-.017(8)
C95	.16(2)	.13(1)	.09(1)	.02(1)	.03(1)	-.03(1)
C96	.13(1)	.08(1)	.08(1)	-.00(1)	.01(1)	-.015(9)
O8	.096(7)	.083(6)	.076(6)	-.015(6)	.013(5)	-.013(5)
P1	.051(2)	.064(2)	.056(2)	-.001(2)	.001(2)	.003(2)
F1	.081(5)	.097(5)	.051(4)	.018(4)	.004(4)	.013(4)
F2	.058(4)	.086(5)	.076(5)	.013(4)	-.004(4)	-.004(4)
F3	.078(5)	.070(4)	.068(4)	-.018(4)	-.011(4)	.003(4)
F4	.059(4)	.089(5)	.085(5)	.010(4)	.008(4)	-.002(4)
F5	.073(5)	.068(5)	.113(6)	-.016(4)	.021(4)	.004(5)
F6	.071(4)	.106(6)	.047(4)	-.007(4)	-.008(4)	-.004(4)
P2	.048(2)	.045(2)	.070(2)	.000(1)	.004(2)	.007(2)
F7	.109(6)	.067(4)	.082(5)	.006(4)	.017(5)	.023(4)
F8	.090(5)	.052(4)	.115(6)	.004(4)	.024(5)	-.009(4)
F9	.049(4)	.101(6)	.141(7)	-.004(4)	-.008(5)	-.005(6)
F10	.107(6)	.061(4)	.085(5)	.022(4)	-.003(5)	-.010(4)
F11	.056(4)	.063(5)	.182(9)	-.006(4)	-.025(5)	.020(5)
F12	.143(7)	.077(5)	.088(5)	-.000(5)	.015(5)	.035(4)
N11	.14(1)	.104(9)	.25(2)	.012(9)	.04(1)	-.05(1)
C97	.14(2)	.34(3)	.11(1)	.07(2)	.03(1)	.10(2)
C98	.14(2)	.15(2)	.17(2)	-.02(2)	.04(2)	.01(2)
N12	.14(2)	.09(3)	.05(1)	-.01(2)	.06(1)	-.00(2)
C99	.10(2)	.14(3)	.05(1)	-.01(2)	.01(1)	-.06(2)
C100	.17(3)	.15(3)	.06(2)	-.09(2)	.02(2)	-.01(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O9	.10(2)	.37(3)	.06(1)	.13(2)	-.04(1)	-.02(2)
C101	.05(2)	.23(3)	.16(1)	-.05(2)	.01(1)	.09(2)
O10	.14(1)	.104(9)	.25(2)	.012(9)	.04(1)	-.05(1)
C102	.10(2)	.37(5)	.06(2)	.13(2)	-.04(2)	-.02(3)
O11	.14(1)	.104(9)	.25(2)	.012(9)	.04(1)	-.05(1)
O12	.14(1)	.104(9)	.25(2)	.012(9)	.04(1)	-.05(1)
C103	.17(2)	.12(1)	.12(1)	.04(1)	-.08(1)	.02(1)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
RU	N1	2.078(8)	N3	C13	1.34(1)
RU	N2	1.961(8)	C13	C14	1.39(2)
RU	N3	2.063(8)	C14	C15	1.38(2)
RU	N6	2.072(8)	C14	C17	1.52(2)
RU	N7	1.968(8)	C15	C16	1.39(2)
RU	N8	2.057(8)	C17	C18	1.53(2)
CU	N4	2.029(9)	C18	C19	1.51(2)
CU	N5	2.043(9)	C19	O1	1.45(2)
CU	N9	2.030(9)	O1	C20	1.36(1)
CU	N10	2.033(9)	C20	C21	1.38(2)
C1	C2	1.51(2)	C20	C25	1.41(2)
C2	C3	1.41(2)	C21	C22	1.38(2)
C2	C6	1.35(2)	C22	C23	1.40(2)
C3	N1	1.32(1)	C23	C24	1.37(2)
N1	C4	1.38(1)	C23	C26	1.47(2)
C4	C5	1.40(2)	C24	C25	1.38(2)
C4	C7	1.46(2)	C26	C27	1.42(2)
C5	C6	1.37(2)	C26	N4	1.38(1)
C7	N2	1.36(1)	C27	C28	1.36(2)
C7	C11	1.38(2)	C28	C29	1.40(2)
N2	C8	1.36(1)	C29	C30	1.44(2)
C8	C9	1.38(2)	C29	C31	1.42(2)
C8	C12	1.46(2)	C30	N4	1.35(1)
C9	C10	1.37(2)	C30	C37	1.41(2)
C10	C11	1.41(2)	C31	C32	1.35(2)
C12	N3	1.36(1)	C32	C33	1.41(2)
C12	C16	1.37(2)	C33	C34	1.40(2)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C33	C37	1.41(2)	C54	C55	1.37(2)
C34	C35	1.36(2)	C55	C56	1.38(1)
C35	C36	1.41(2)	C56	N7	1.36(1)
C36	N5	1.33(1)	C56	C57	1.49(2)
C36	C38	1.46(1)	C57	C58	1.38(2)
N5	C37	1.38(1)	C57	N8	1.36(1)
C38	C39	1.39(2)	C58	C59	1.37(2)
C38	C43	1.40(2)	C59	C60	1.37(2)
C39	C40	1.38(2)	C60	C61	1.38(2)
C40	C41	1.38(2)	C60	C62	1.51(2)
C41	C42	1.39(2)	C61	N8	1.34(1)
C41	O2	1.35(1)	C63	C64	1.40(2)
C42	C43	1.36(2)	C63	C68	1.37(2)
O2	C44	1.45(1)	C63	O8	1.39(2)
C44	C45	1.51(2)	C64	C65	1.37(2)
C45	C46	1.52(2)	C65	C66	1.39(2)
C46	C47	1.51(2)	C66	C67	1.39(2)
C47	C48	1.37(2)	C66	C69	1.47(2)
C47	C51	1.37(2)	C67	C68	1.39(2)
C48	C49	1.39(2)	C69	C70	1.40(2)
C49	C50	1.36(2)	C69	N9	1.36(2)
C50	N6	1.38(1)	C70	C71	1.34(2)
C50	C52	1.46(1)	C71	C72	1.41(2)
N6	C51	1.33(1)	C72	C73	1.43(2)
C52	C53	1.37(1)	C72	C74	1.43(2)
C52	N7	1.36(1)	C73	N9	1.34(1)
C53	C54	1.40(2)	C73	C77	1.42(2)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C74	C75	1.31(2)	C94	O7	1.49(3)
C75	C76	1.44(2)	O7	C95	1.28(2)
C76	C77	1.38(2)	C95	C96	1.48(3)
C76	C80	1.40(2)	C96	O8	1.40(2)
C77	N10	1.37(1)	P1	F1	1.588(8)
N10	C78	1.36(2)	P1	F2	1.601(8)
C78	C79	1.43(2)	P1	F3	1.594(8)
C78	C81	1.49(2)	P1	F4	1.597(8)
C79	C80	1.36(2)	P1	F5	1.594(8)
C81	C82	1.35(2)	P1	F6	1.607(8)
C81	C86	1.40(2)	P2	F7	1.580(9)
C82	C83	1.36(2)	P2	F8	1.580(8)
C83	C84	1.40(2)	P2	F9	1.572(8)
C84	C85	1.37(2)	P2	F10	1.592(8)
C84	O3	1.36(2)	P2	F11	1.570(8)
C85	C86	1.39(2)	P2	F12	1.582(9)
O3	C87	1.45(2)	P3	F13	1.59(2)
C87	C88	1.44(3)	P3	F14	1.50(2)
C88	O4	1.41(3)	P3	F15	1.61(2)
O4	C89	1.46(2)	P3	F16	1.60(2)
C89	C90	1.39(3)	P3	F17	1.59(2)
C90	O5	1.20(3)	P3	F18	1.51(2)
O5	C91	1.47(3)	F13	F15	2.18(2)
C91	C92	1.48(3)	F13	F16	2.16(2)
C92	O6	1.31(3)	F16	F17	2.17(2)
O6	C93	1.52(4)	F16	F18	2.18(3)
C93	C94	1.34(4)	N11	C97	1.19(4)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C97	C98	1.37(4)	O9	C101	1.50(5)
N12	C99	1.18(5)	O10	C102	1.67(5)
C99	C100	1.63(5)	O12	C103	1.09(3)

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
N1	RU	N2	79.8(3)	C3	N1	C4	119.0(9)
N1	RU	N3	158.4(3)	N1	C4	C5	118(1)
N1	RU	N6	87.9(3)	N1	C4	C7	116.2(9)
N1	RU	N7	97.3(3)	C5	C4	C7	124(1)
N1	RU	N8	94.5(3)	C4	C5	C6	120(1)
N2	RU	N3	78.6(3)	C2	C6	C5	120(1)
N2	RU	N6	101.7(3)	C4	C7	N2	112.6(9)
N2	RU	N7	176.8(3)	C4	C7	C11	126(1)
N2	RU	N8	99.4(3)	N2	C7	C11	120(1)
N3	RU	N6	96.8(3)	RU	N2	C7	119.1(7)
N3	RU	N7	104.3(3)	RU	N2	C8	119.6(7)
N3	RU	N8	88.6(3)	C7	N2	C8	121.3(9)
N6	RU	N7	79.3(3)	N2	C8	C9	120(1)
N6	RU	N8	158.8(3)	N2	C8	C12	112.1(9)
N7	RU	N8	79.5(3)	C9	C8	C12	127(1)
N4	CU	N5	82.9(4)	C8	C9	C10	118(1)
N4	CU	N9	133.5(3)	C9	C10	C11	121(1)
N4	CU	N10	111.6(4)	C7	C11	C10	117(1)
N5	CU	N9	118.0(4)	C8	C12	N3	115(1)
N5	CU	N10	137.1(3)	C8	C12	C16	123(1)
N9	CU	N10	81.9(4)	N3	C12	C16	121(1)
C1	C2	C3	119(1)	RU	N3	C12	114.6(7)
C1	C2	C6	123(1)	RU	N3	C13	128.2(7)
C3	C2	C6	116(1)	C12	N3	C13	117.1(9)
C2	C3	N1	124(1)	N3	C13	C14	125(1)
RU	N1	C3	128.6(7)	C13	C14	C15	115(1)
RU	N1	C4	112.3(7)	C13	C14	C17	120(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle
C15	C14	C17	123(1)
C14	C15	C16	120(1)
C12	C16	C15	119(1)
C14	C17	C18	116(1)
C17	C18	C19	112(1)
C18	C19	O1	106(1)
C19	O1	C20	118(1)
O1	C20	C21	125(1)
O1	C20	C25	115(1)
C21	C20	C25	119(1)
C20	C21	C22	119(1)
C21	C22	C23	120(1)
C22	C23	C24	119(1)
C22	C23	C26	121(1)
C24	C23	C26	119(1)
C23	C24	C25	121(1)
C20	C25	C24	119(1)
C23	C26	C27	121(1)
C23	C26	N4	117(1)
C27	C26	N4	120(1)
C26	C27	C28	119(1)
C27	C28	C29	121(1)
C28	C29	C30	116(1)
C28	C29	C31	125(1)
C30	C29	C31	118(1)
C29	C30	N4	122(1)
C29	C30	C37	119(1)
N4	C30	C37	118(1)
CU	N4	C26	129.1(7)
CU	N4	C30	111.1(7)
C26	N4	C30	119.3(9)
C29	C31	C32	121(1)
C31	C32	C33	120(1)
C32	C33	C34	123(1)
C32	C33	C37	119(1)
C34	C33	C37	116(1)
C33	C34	C35	119(1)
C34	C35	C36	121(1)
C35	C36	N5	120(1)
C35	C36	C38	120(1)
N5	C36	C38	119.7(9)
CU	N5	C36	130.7(7)
CU	N5	C37	109.8(7)
C36	N5	C37	119.0(9)
C30	C37	C33	119(1)
C30	C37	N5	117(1)
C33	C37	N5	122(1)
C36	C38	C39	122(1)
C36	C38	C43	121(1)
C39	C38	C43	116(1)
C38	C39	C40	122(1)
C39	C40	C41	119(1)
C40	C41	C42	119(1)
C40	C41	O2	126(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C42	C41	O2	114(1)	N7	C56	C57	112.2(9)
C41	C42	C43	119(1)	RU	N7	C52	119.1(7)
C38	C43	C42	122(1)	RU	N7	C56	118.9(7)
C41	O2	C44	118.1(9)	C52	N7	C56	121.4(9)
O2	C44	C45	110.8(9)	C56	C57	C58	123(1)
C44	C45	C46	110.3(9)	C56	C57	N8	114.8(9)
C45	C46	C47	117(1)	C58	C57	N8	122(1)
C46	C47	C48	122(1)	C57	C58	C59	118(1)
C46	C47	C51	120(1)	C58	C59	C60	120(1)
C48	C47	C51	116(1)	C59	C60	C61	117(1)
C47	C48	C49	119(1)	C59	C60	C62	122(1)
C48	C49	C50	121(1)	C61	C60	C62	120(1)
C49	C50	N6	119.0(9)	C60	C61	N8	124(1)
C49	C50	C52	125(1)	RU	N8	C57	114.4(7)
N6	C50	C52	116.0(9)	RU	N8	C61	128.5(7)
RU	N6	C50	112.8(6)	C57	N8	C61	117.1(9)
RU	N6	C51	128.2(7)	C64	C63	C68	118(1)
C50	N6	C51	118.9(9)	C64	C63	O8	116(1)
C47	C51	N6	124(1)	C68	C63	O8	124(1)
C50	C52	C53	127(1)	C63	C64	C65	122(1)
C50	C52	N7	112.4(9)	C64	C65	C66	119(1)
C53	C52	N7	119.6(9)	C65	C66	C67	118(1)
C52	C53	C54	119(1)	C65	C66	C69	121(1)
C53	C54	C55	120(1)	C67	C66	C69	120(1)
C54	C55	C56	118(1)	C66	C67	C68	122(1)
C55	C56	N7	120(1)	C63	C68	C67	118(1)
C55	C56	C57	127.4(9)	C66	C69	C70	121(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C66	C69	N9	117(1)	C78	C79	C80	118(1)
C70	C69	N9	120(1)	C76	C80	C79	122(1)
C69	C70	C71	119(1)	C78	C81	C82	121(1)
C70	C71	C72	122(1)	C78	C81	C86	120(1)
C71	C72	C73	115(1)	C82	C81	C86	118(1)
C71	C72	C74	127(1)	C81	C82	C83	123(1)
C73	C72	C74	116(1)	C82	C83	C84	118(1)
C72	C73	N9	121(1)	C83	C84	C85	119(1)
C72	C73	C77	119(1)	C83	C84	O3	122(1)
N9	C73	C77	118(1)	C85	C84	O3	118(1)
CU	N9	C69	128.6(8)	C84	C85	C86	121(1)
CU	N9	C73	111.5(8)	C81	C86	C85	119(1)
C69	N9	C73	119(1)	C84	O3	C87	118(1)
C72	C74	C75	123(1)	O3	C87	C88	112(1)
C74	C75	C76	120(1)	C87	C88	O4	106(1)
C75	C76	C77	119(1)	C88	O4	C89	110(1)
C75	C76	C80	124(1)	O4	C89	C90	114(1)
C77	C76	C80	116(1)	C89	C90	O5	120(2)
C73	C77	C76	120(1)	C90	O5	C91	116(1)
C73	C77	N10	116(1)	O5	C91	C92	109(1)
C76	C77	N10	123(1)	C91	C92	O6	108(1)
CU	N10	C77	111.5(7)	C92	O6	C93	120(1)
CU	N10	C78	128.9(8)	O6	C93	C94	102(2)
C77	N10	C78	118(1)	C93	C94	O7	109(2)
N10	C78	C79	120(1)	C94	O7	C95	116(1)
N10	C78	C81	115(1)	O7	C95	C96	112(1)
C79	C78	C81	123(1)	C95	C96	O8	109(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
C63	O8	C96	117(1)	F9	P2	F12	89.6(5)
F1	P1	F2	89.9(4)	F10	P2	F11	88.8(5)
F1	P1	F3	90.4(4)	F10	P2	F12	90.9(5)
F1	P1	F4	90.8(4)	F11	P2	F12	91.3(5)
F1	P1	F5	90.5(5)	F13	P3	F14	91(1)
F1	P1	F6	179.6(5)	F13	P3	F15	85.5(9)
F2	P1	F3	90.7(4)	F13	P3	F16	85.3(9)
F2	P1	F4	179.2(4)	F13	P3	F17	88(1)
F2	P1	F5	89.0(4)	F13	P3	F18	172(1)
F2	P1	F6	89.7(4)	F14	P3	F15	92.0(9)
F3	P1	F4	89.8(4)	F14	P3	F16	177(1)
F3	P1	F5	179.1(4)	F14	P3	F17	93.5(9)
F3	P1	F6	89.5(4)	F14	P3	F18	94(1)
F4	P1	F5	90.5(4)	F15	P3	F16	88.2(8)
F4	P1	F6	89.6(4)	F15	P3	F17	172.0(9)
F5	P1	F6	89.7(4)	F15	P3	F18	89(1)
F7	P2	F8	91.2(5)	F16	P3	F17	86.0(9)
F7	P2	F9	88.8(5)	F16	P3	F18	88(1)
F7	P2	F10	88.5(4)	F17	P3	F18	95(1)
F7	P2	F11	90.3(5)	P3	F13	F15	47.6(7)
F7	P2	F12	178.3(5)	P3	F13	F16	47.4(7)
F8	P2	F9	89.3(5)	F15	F13	F16	62.0(8)
F8	P2	F10	179(1)	P3	F15	F13	46.9(7)
F8	P2	F11	91.1(5)	P3	F16	F13	47.3(7)
F8	P2	F12	89.4(5)	P3	F16	F17	46.8(6)
F9	P2	F10	90.7(5)	P3	F16	F18	43.9(7)
F9	P2	F11	179.0(5)	F13	F16	F17	61.6(8)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
F13	F16	F18	91.1(9)	P3	F18	F16	47.2(8)
F17	F16	F18	63.9(8)	N11	C97	C98	169(2)
P3	F17	F16	47.2(6)	N12	C99	C100	176(3)

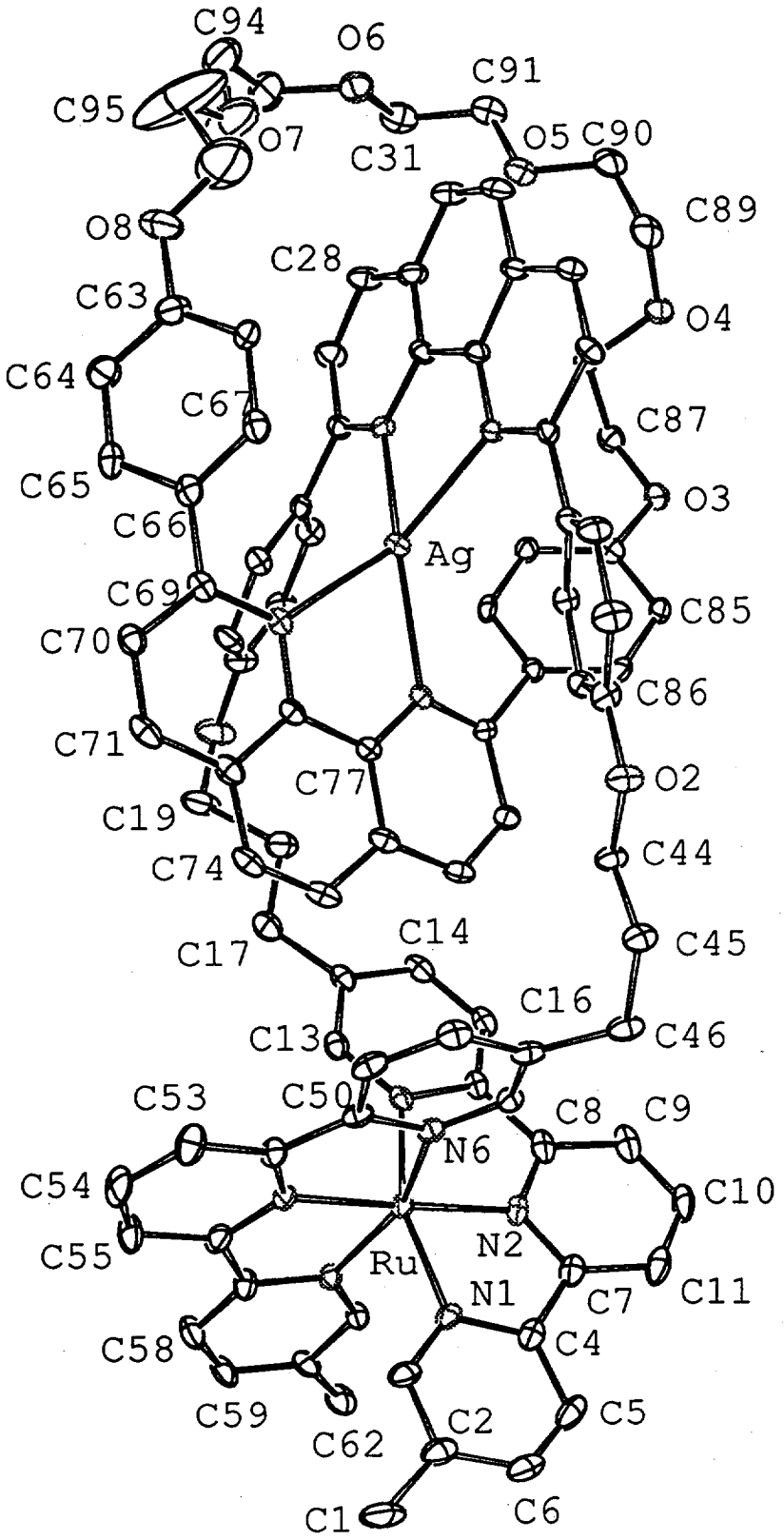
C94
O6
C91
C95
O7
C31
O5
C90
C89
O8
C28
C63
O4
C64
C67
C87
C65
O3
C66
Ag
C69
C85
C70
C86
C71
C77
O2
C19
C44
C74
C14
C45
C17
C16
C46
C13
C53
C50
C8
C9
N6
C54
C10
C55
N2
Ru
C7
C11
N1
C58
C4
C59
C2
C5
C62
C1
C6

Table 1 : X-ray experimental data

Formula	: $C_{126}H_{120}N_{10}O_{11}F_{18}P_3RuAg$
Molecular weight	: 2594.25
Crystal system	: triclinic
Space group	: P-1
a(Å)	: 17.742(2)
b(Å)	: 18.815(2)
c(Å)	: 21.564(2)
α(deg)	: 112.265(7)
β(deg)	: 103.620(7)
γ(deg)	: 97.633(7)
V(Å^3)	: 6273(2)
Z	: 2
Color	: dark red
Crystal dim(mm)	: 0.40*0.40*0.40
Dcalc(gcm^{-3})	: 1.37
F000	: 2664
μ(mm^{-1})	: 0.394
Trans. min and max	: 0.94/1.00
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphite monochromated
Scan mode	: θ/2θ
hkl limits	: -20,20/-22,20/0,25
Theta limits(deg)	: 2.5/24.63
Weighting scheme	: $4Fo^2/(\sigma^2(Fo^2) + 0.0064\ Fo^4)$
Number of data meas.	: 21820
Number of data with I > 3 σ(I)	: 11068
Number of variables	: 1412
R	: 0.068
Rw	: 0.097
GOF	: 1.800
Largest peak in final difference (eÅ^{-3})	: 0.417

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
RU	-0.03727(4)	-0.20326(4)	0.18275(3)	0.0283(3)
AG	0.45300(4)	0.17347(4)	0.21408(3)	0.0346(3)
C1	-0.1230(7)	-0.4826(6)	0.2114(6)	0.071(6)
C2	-0.1273(5)	-0.4413(6)	0.1627(6)	0.049(5)
C3	-0.0892(5)	-0.3628(5)	0.1880(5)	0.042(5)
N1	-0.0890(4)	-0.3211(4)	0.1487(4)	0.032(3)
C4	-0.1285(5)	-0.3600(6)	0.0785(5)	0.039(5)
C5	-0.1695(6)	-0.4412(6)	0.0493(6)	0.050(6)
C6	-0.1672(6)	-0.4785(6)	0.0908(6)	0.049(5)
C7	-0.1258(5)	-0.3100(6)	0.0397(5)	0.038(5)
N2	-0.0896(4)	-0.2341(4)	0.0823(3)	0.030(3)
C8	-0.0800(5)	-0.1799(5)	0.0561(4)	0.039(4)
C9	-0.1083(5)	-0.2039(6)	-0.0172(5)	0.049(5)
C10	-0.1441(6)	-0.2802(7)	-0.0609(5)	0.045(5)
C11	-0.1541(6)	-0.3332(7)	-0.0341(5)	0.049(6)
C12	-0.0353(5)	-0.1000(5)	0.1109(4)	0.036(4)
N3	-0.0078(4)	-0.0958(4)	0.1779(3)	0.033(3)
C13	0.0331(5)	-0.0257(5)	0.2304(4)	0.039(4)
C14	0.0500(5)	0.0446(5)	0.2217(4)	0.043(4)
C15	0.0208(5)	0.0381(5)	0.1540(4)	0.055(5)
C16	-0.0221(5)	-0.0340(5)	0.0994(4)	0.046(4)
C17	0.0953(6)	0.1204(6)	0.2852(5)	0.061(5)
C18	0.1317(6)	0.1889(6)	0.2725(5)	0.057(5)
C19	0.1715(7)	0.2613(6)	0.3405(6)	0.075(6)
O1	0.1983(4)	0.3274(4)	0.3271(4)	0.074(4)
C20	0.2689(5)	0.3346(5)	0.3119(5)	0.047(5)
C21	0.3286(6)	0.3009(5)	0.3297(4)	0.056(5)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C22	0.3989(5)	0.3115(5)	0.3116(4)	0.043(4)
C23	0.4073(5)	0.3559(5)	0.2740(4)	0.030(4)
C24	0.3458(5)	0.3913(5)	0.2568(5)	0.045(4)
C25	0.2777(5)	0.3803(5)	0.2751(5)	0.047(5)
C26	0.4778(5)	0.3626(5)	0.2491(4)	0.035(4)
C27	0.5153(6)	0.4355(5)	0.2550(5)	0.051(5)
C28	0.5810(6)	0.4422(5)	0.2334(5)	0.053(5)
C29	0.6085(5)	0.3747(5)	0.2036(5)	0.043(4)
C30	0.5662(5)	0.3033(5)	0.1969(4)	0.035(4)
N4	0.5026(4)	0.2975(4)	0.2213(3)	0.030(3)
C31	0.6770(5)	0.3784(5)	0.1814(5)	0.050(5)
C32	0.7029(5)	0.3129(6)	0.1522(5)	0.049(5)
C33	0.6590(5)	0.2371(5)	0.1397(4)	0.040(4)
C34	0.6807(5)	0.1669(5)	0.1058(4)	0.041(4)
C35	0.6350(5)	0.0966(5)	0.0927(4)	0.044(4)
C36	0.5675(5)	0.0939(5)	0.1162(4)	0.030(4)
N5	0.5469(4)	0.1589(4)	0.1511(3)	0.029(3)
C37	0.5909(5)	0.2312(5)	0.1621(4)	0.034(4)
C38	0.5158(4)	0.0164(5)	0.1003(4)	0.035(4)
C39	0.4339(5)	0.0065(5)	0.0919(4)	0.036(4)
C40	0.3859(5)	-0.0626(5)	0.0805(4)	0.036(4)
C41	0.4187(5)	-0.1288(5)	0.0745(5)	0.040(4)
C42	0.4992(5)	-0.1201(5)	0.0818(5)	0.050(5)
C43	0.5467(5)	-0.0497(5)	0.0938(5)	0.043(4)
O2	0.3762(3)	-0.2008(3)	0.0623(3)	0.044(3)
C44	0.2945(5)	-0.2099(5)	0.0610(5)	0.040(4)
C45	0.2651(5)	-0.2963(5)	0.0451(5)	0.043(5)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C46	0.1787(5)	-0.3165(5)	0.0448(5)	0.044(5)
C47	0.1650(5)	-0.2769(5)	0.1147(5)	0.038(4)
C48	0.2191(5)	-0.2626(5)	0.1791(5)	0.046(5)
C49	0.1993(5)	-0.2317(5)	0.2391(5)	0.040(5)
C50	0.1238(5)	-0.2138(5)	0.2382(4)	0.036(4)
N6	0.0711(4)	-0.2265(4)	0.1748(3)	0.033(3)
C51	0.0928(5)	-0.2559(5)	0.1167(4)	0.032(4)
C52	0.0962(5)	-0.1830(5)	0.2995(4)	0.037(4)
C53	0.1383(6)	-0.1643(6)	0.3672(5)	0.056(6)
C54	0.1001(7)	-0.1369(7)	0.4175(5)	0.056(6)
C55	0.0222(7)	-0.1291(7)	0.4017(5)	0.057(6)
C56	-0.0175(6)	-0.1512(5)	0.3302(5)	0.041(5)
N7	0.0208(4)	-0.1750(4)	0.2821(3)	0.031(3)
C57	-0.1012(5)	-0.1505(5)	0.3004(4)	0.039(4)
C58	-0.1536(6)	-0.1333(6)	0.3378(5)	0.057(5)
C59	-0.2314(6)	-0.1350(6)	0.3044(5)	0.060(5)
C60	-0.2567(5)	-0.1557(5)	0.2329(4)	0.046(4)
C61	-0.1996(5)	-0.1740(5)	0.1978(4)	0.038(4)
C62	-0.3386(6)	-0.1560(7)	0.1944(5)	0.063(5)
N8	-0.1248(4)	-0.1725(4)	0.2287(3)	0.032(3)
C63	0.6849(6)	0.3692(6)	0.4037(5)	0.059(6)
C64	0.6437(6)	0.3779(6)	0.4532(5)	0.056(6)
C65	0.5866(6)	0.3143(6)	0.4452(5)	0.049(5)
C66	0.5682(5)	0.2411(5)	0.3871(4)	0.042(4)
C67	0.6134(5)	0.2330(5)	0.3400(5)	0.046(5)
C68	0.6728(6)	0.2973(6)	0.3493(5)	0.043(5)
C69	0.5005(5)	0.1781(5)	0.3741(4)	0.042(4)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C70	0.4915(5)	0.1571(5)	0.4274(4)	0.047(5)
C71	0.4271(6)	0.0977(5)	0.4139(4)	0.064(5)
C72	0.3701(5)	0.0606(5)	0.3471(4)	0.047(4)
C73	0.3816(5)	0.0872(5)	0.2963(4)	0.037(4)
N9	0.4476(4)	0.1434(4)	0.3096(3)	0.035(3)
C74	0.3011(6)	-0.0003(5)	0.3288(4)	0.060(5)
C75	0.2457(5)	-0.0309(5)	0.2659(5)	0.058(4)
C76	0.2516(5)	-0.0019(5)	0.2152(4)	0.042(4)
C77	0.3190(5)	0.0591(4)	0.2307(4)	0.030(4)
N10	0.3244(4)	0.0929(3)	0.1860(3)	0.028(3)
C78	0.2661(4)	0.0706(4)	0.1275(4)	0.028(4)
C79	0.1985(5)	0.0076(5)	0.1061(4)	0.037(4)
C80	0.1919(5)	-0.0286(5)	0.1492(5)	0.044(4)
C81	0.2737(5)	0.1144(5)	0.0830(4)	0.031(4)
C82	0.3071(5)	0.1968(5)	0.1182(4)	0.029(4)
C83	0.3218(5)	0.2406(5)	0.0816(4)	0.033(4)
C84	0.3032(5)	0.2030(5)	0.0096(4)	0.036(4)
C85	0.2686(5)	0.1219(5)	-0.0263(4)	0.033(4)
C86	0.2543(5)	0.0784(5)	0.0103(4)	0.031(4)
O3	0.3144(4)	0.2411(3)	-0.0321(3)	0.044(3)
C87	0.3448(5)	0.3258(5)	0.0014(4)	0.046(4)
C88	0.4341(5)	0.3535(5)	0.0330(4)	0.041(4)
O4	0.4677(3)	0.3372(4)	-0.0219(3)	0.046(3)
C89	0.5512(6)	0.3582(6)	-0.0005(5)	0.062(5)
C90	0.5900(5)	0.4438(6)	0.0261(5)	0.057(5)
O5	0.5948(4)	0.4883(3)	0.0985(3)	0.055(3)
C91	0.6278(6)	0.5699(6)	0.1222(5)	0.066(5)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
C92	0.6356(6)	0.6145(6)	0.1969(6)	0.066(6)	
O6	0.6978(4)	0.6007(4)	0.2416(3)	0.059(4)	
C93	0.7075(9)	0.6458(8)	0.3156(7)	0.084(9)	
C94	0.773(1)	0.6297(8)	0.3599(7)	0.095(9)	
O7	0.7478(7)	0.5507(6)	0.3538(5)	0.143(7)	
C95	0.800(2)	0.538(1)	0.400(1)	0.35(1)	
C96	0.774(1)	0.437(1)	0.3690(9)	0.18(1)	
O8	0.7378(5)	0.4351(5)	0.4141(4)	0.088(5)	
P1	0.0860(1)	-0.1792(1)	-0.0773(1)	0.046(1)	
F1	0.0964(4)	-0.1555(4)	-0.1382(3)	0.100(3)	
F2	0.1198(3)	-0.2552(3)	-0.1083(3)	0.063(3)	
F3	-0.0019(3)	-0.2283(4)	-0.1226(3)	0.064(4)	
F4	0.1755(3)	-0.1274(3)	-0.0315(3)	0.063(3)	
F5	0.0532(3)	-0.1025(3)	-0.0440(3)	0.061(3)	
F6	0.0779(4)	-0.2001(3)	-0.0137(3)	0.088(3)	
P2	0.3403(2)	-0.4398(1)	0.1609(2)	0.049(1)	
F7	0.2560(4)	-0.4353(4)	0.1165(4)	0.077(4)	
F8	0.3332(5)	-0.3753(6)	0.2266(5)	0.120(6)	
F9	0.2949(6)	-0.5107(5)	0.1644(5)	0.167(6)	
F10	0.3842(6)	-0.3727(4)	0.1486(4)	0.142(5)	
F11	0.3441(5)	-0.4990(6)	0.0876(5)	0.135(6)	
F12	0.4203(4)	-0.4447(4)	0.2037(4)	0.105(4)	
P3	0.1914(2)	0.0966(2)	0.4766(1)	0.071(2)	
F13	0.2351	0.1616	0.5524	0.111(3)	*
F14	0.1478	0.0316	0.4009	0.093(2)	*
F15	0.1441	0.0493	0.5065	0.105(5)	*
F16	0.2387	0.1439	0.4467	0.069(4)	*

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
F17	0.1246	0.1411	0.4696	0.128(6)	*
F18	0.2583	0.0521	0.4836	0.118(6)	*
F19	0.1047	0.0847	0.4875	0.087(4)	*
F20	0.2030	0.0357	0.5119	0.092(5)	*
F21	0.1814	0.1661	0.4510	0.136(7)	*
F22	0.2847	0.1003	0.4743	0.161(8)	*
C97	0.0248(9)	0.4189(9)	0.1255(8)	0.104(5)	*
C98	0.025(1)	0.4724(9)	0.0900(8)	0.120(6)	*
C99	0.074(1)	0.545(1)	0.141(1)	0.148(7)	*
C100	0.111(1)	0.561(1)	0.210(1)	0.160(8)	*
C101	0.109(1)	0.504(1)	0.241(1)	0.155(8)	*
C102	0.0600(9)	0.4303(9)	0.1886(8)	0.110(5)	*
C103	0.7875(9)	0.076(1)	0.2240(9)	0.14(1)	
C104	0.7321(9)	0.086(1)	0.2586(8)	0.13(1)	
C105	0.741(1)	0.079(1)	0.3174(9)	0.13(1)	
C106	0.807(2)	0.064(1)	0.3527(9)	0.18(1)	
C107	0.873(1)	0.0586(9)	0.3218(8)	0.13(1)	
C108	0.8570(8)	0.0582(9)	0.256(1)	0.13(1)	
C109	0.4845(7)	-0.0940(7)	0.2682(6)	0.086(7)	
C110	0.4674(7)	-0.1751(8)	0.2406(6)	0.068(7)	
C111	0.5096(7)	-0.2107(7)	0.2773(6)	0.076(7)	
C112	0.5697(7)	-0.1636(7)	0.3415(6)	0.080(7)	
C113	0.5881(7)	-0.0844(7)	0.3672(6)	0.065(7)	
C114	0.5442(7)	-0.0482(7)	0.3313(7)	0.076(7)	
C115	0.3568(8)	-0.2302(8)	0.3820(7)	0.095(8)	
C116	0.3803(7)	-0.1503(8)	0.4061(6)	0.089(7)	
C117	0.3620(7)	-0.1006(7)	0.4622(6)	0.070(6)	

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv	
C118	0.3210(6)	-0.1282(6)	0.4960(5)	0.065(6)	
C119	0.2970(7)	-0.2073(8)	0.4728(6)	0.099(7)	
C120	0.3131(8)	-0.2624(7)	0.4136(8)	0.091(8)	
C121	0.5155(9)	-0.3349(8)	0.4060(7)	0.099(5)	*
C122	0.465(1)	-0.4023(9)	0.3896(8)	0.118(6)	*
C123	0.489(1)	-0.446(1)	0.4245(9)	0.129(6)	*
C124	0.569(1)	-0.430(1)	0.463(1)	0.174(9)	*
C125	0.625(2)	-0.358(1)	0.480(1)	0.21(1)	*
C126	0.587(1)	-0.3096(9)	0.4496(8)	0.118(6)	*
O9	0.057(2)	0.662(1)	0.711(1)	0.16(1)	*
O10	0.227(3)	0.050(3)	0.876(2)	0.31(2)	*
O11	0.026(2)	0.419(2)	0.387(2)	0.21(1)	*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor. Starred atoms were refined isotropically.

Table of Positional Parameters

Atom	x	y	z	Ueqv	
H1	-0.1525	-0.5363	0.1851	0.1014	*
H2	-0.0687	-0.4806	0.2320	0.1014	*
H3	-0.1451	-0.4567	0.2475	0.1014	*
H4	-0.0608	-0.3355	0.2369	0.0615	*
H5	-0.1984	-0.4686	0.0004	0.0811	*
H6	-0.1939	-0.5331	0.0703	0.0769	*
H7	-0.1021	-0.1660	-0.0359	0.0699	*
H8	-0.1622	-0.2965	-0.1105	0.0762	*
H9	-0.1805	-0.3870	-0.0649	0.0856	*
H10	0.0520	-0.0230	0.2765	0.0495	*
H11	0.0304	0.0836	0.1450	0.0634	*
H12	-0.0427	-0.0376	0.0532	0.0588	*
H13	0.1376	0.1087	0.3130	0.0739	*
H14	0.0594	0.1374	0.3109	0.0739	*
H15	0.0906	0.2006	0.2434	0.0748	*
H16	0.1703	0.1743	0.2493	0.0748	*
H17	0.2160	0.2516	0.3676	0.1009	*
H18	0.1343	0.2730	0.3660	0.1009	*
H19	0.3227	0.2696	0.3548	0.0654	*
H20	0.4405	0.2883	0.3251	0.0531	*
H21	0.3514	0.4232	0.2322	0.0556	*
H22	0.2361	0.4040	0.2625	0.0608	*
H23	0.4951	0.4806	0.2741	0.0645	*
H24	0.6079	0.4922	0.2385	0.0674	*
H25	0.7056	0.4280	0.1871	0.0661	*
H26	0.7507	0.3174	0.1399	0.0647	*
H27	0.7278	0.1689	0.0920	0.0547	*

Table of Positional Parameters (cont.)

Atom	x	y	z	Ueqv	
H28	0.6482	0.0489	0.0676	0.0539	*
H29	0.4110	0.0499	0.0942	0.0453	*
H30	0.3308	-0.0666	0.0766	0.0474	*
H31	0.5221	-0.1638	0.0784	0.0672	*
H32	0.6017	-0.0456	0.0977	0.0587	*
H33	0.2643	-0.1979	0.0253	0.0550	*
H34	0.2908	-0.1763	0.1054	0.0550	*
H35	0.2985	-0.3074	0.0800	0.0595	*
H36	0.2684	-0.3284	0.0000	0.0595	*
H37	0.1622	-0.3722	0.0294	0.0628	*
H38	0.1464	-0.3014	0.0124	0.0628	*
H39	0.2698	-0.2745	0.1809	0.0611	*
H40	0.2367	-0.2219	0.2828	0.0593	*
H41	0.0563	-0.2630	0.0735	0.0432	*
H42	0.1916	-0.1698	0.3795	0.0806	*
H43	0.1288	-0.1227	0.4653	0.0893	*
H44	-0.0028	-0.1099	0.4371	0.0843	*
H45	-0.1368	-0.1201	0.3868	0.0744	*
H46	-0.2673	-0.1219	0.3310	0.0745	*
H47	-0.2156	-0.1885	0.1485	0.0497	*
H48	-0.3689	-0.1423	0.2262	0.0809	*
H49	-0.3348	-0.1185	0.1750	0.0809	*
H50	-0.3642	-0.2073	0.1576	0.0809	*
H51	0.6550	0.4276	0.4925	0.0781	*
H52	0.5597	0.3206	0.4795	0.0693	*
H53	0.6037	0.1832	0.3012	0.0604	*
H54	0.7039	0.2906	0.3181	0.0662	*