ORGANIC LETTERS

An Extremely Stable Interwoven Supramolecular Bundle

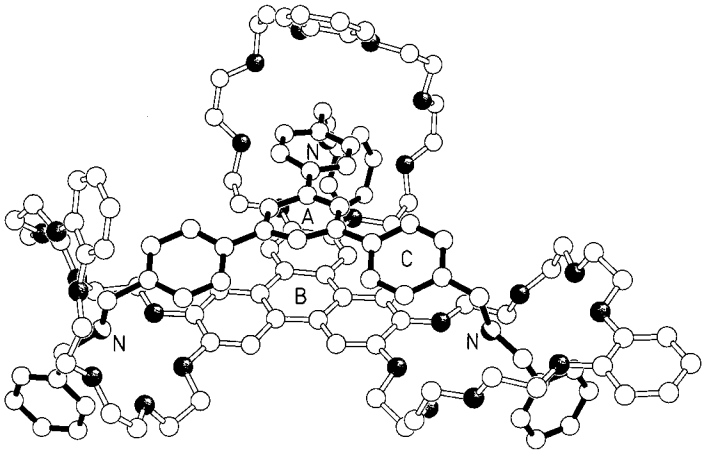
Matthew C. T. Fyfe, James N. Lowe, J. Fraser Stoddart,
and David J. Williams

SUPPORTING INFORMATION
(21 PAGES)

EXPERIMENTAL PROCEDURES FOR **2** AND **3**·3PF_6

^{1}H NMR CD_3SOCD_3 ADDITION EXPERIMENT WITH **2** AND **3**·3PF_6

CRYSTAL DATA FOR [**1**·**2**]$^{3+}$



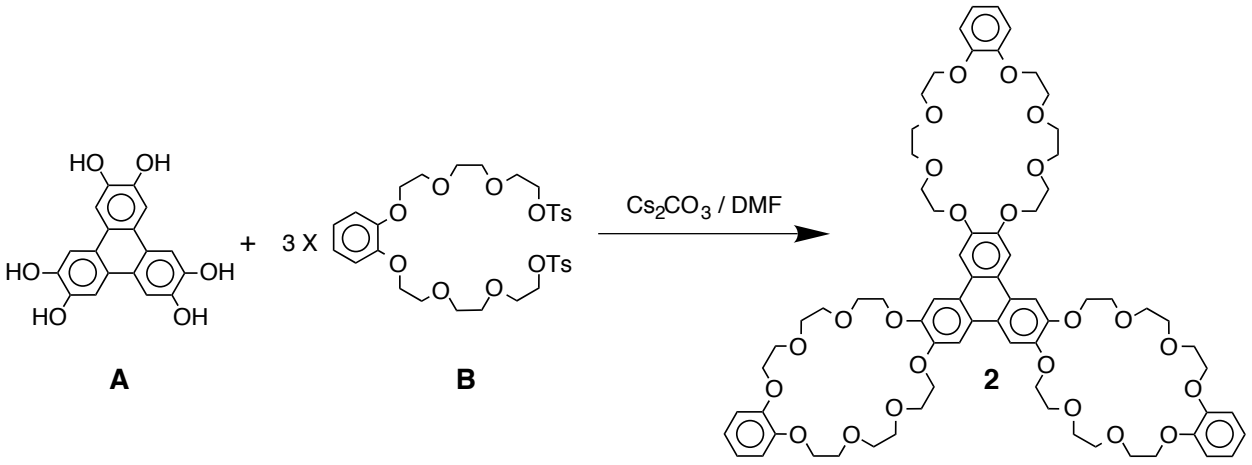
Experimental Section

General

All reagents and solvents were used as received unless otherwise stated. Reactions were carried out under an atmosphere of anhydrous argon. Reactions were monitored by TLC on silica plates (Merck, 0.25 mm) and visualized with UV light (254 nm). Melting points given are uncorrected. NMR Spectra were recorded on either a Bruker AMX 400 or AMX 500 spectrometer. Chemical shifts reported are referenced to the residual solvent peak. NMR Solvents CD_3CN and $CDCl_3$ were stored over 4 Å molecular sieves.

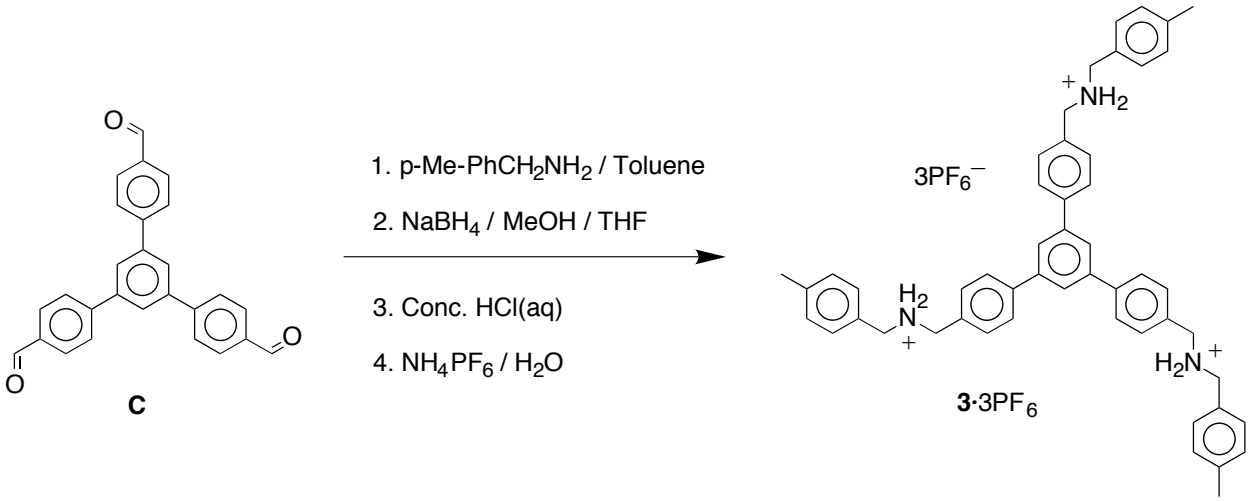
Synthesis

Triscrown 2: An oven dried 2 L three-necked round-bottomed flask was equipped with a stirrer bar, nitrogen inlet, addition funnel and condenser. The flask was purged with argon for 10 min and then charged with 300 mL of anhydrous DMF. Cesium carbonate (30.1 g, 92 mmol) was added to the flask. The white suspension was stirred vigorously and heated to 100°C. The addition funnel was charged with a solution of 2,3,6,7,10,11-hexahydroxytriphenylene[1] **A** (2.5 g, 7.7 mmol) and bistosylate[2] **B** (15.8 g, 23 mmol) in 500 mL of anhydrous DMF. The solution was added dropwise over 24 hours to the suspension. The suspension was heated under reflux for an additional 6 days. Upon cooling down to ambient temperature, the suspension was filtered through a celite pad. The residue was washed with $CHCl_3$ (250 mL). The filtrate and $CHCl_3$ wash was concentrated under reduced pressure. The resulting dark tar was dissolved in CH_2Cl_2 (500 mL) and washed with 10% w/v $K_2CO_{3(aq)}$ (2 x 300 mL) and H_2O (300 mL). The organic layer was dried over $MgSO_4$. The mixture was filtered, concentrated under reduced pressure, and dried to afford a black tar. This tar was subjected to succesive silica gel column chromatography (eluent: 25/1 *i*-PrOH/$CHCl_3$ to 4/1 *i*-PrOH/$CHCl_3$) until pure crown was isolated to afford compound **2** as an off-white solid. (1.03 g, 10 %). FABMS *m/z* = 1338 [M^+]; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.87-3.94 (m, 36H) 4.03 (m, 12H) 4.15 (m, 12H) 4.39 (m, 12H) 6.85 (m, 12H), 7.80 (s, 6H); ^{13}C NMR ($CDCl_3$) δ 69.3, 69.8, 70.0, 71.3, 71.3, 107.4, 114.1, 121.4, 123.8, 148.7, 148.9.



Trimethyltrisammonium salt 3·3PF_6: A mixture of 1,3,5-tris(4-formylphenyl)benzene[3] **C** (100 mg, 0.26 mmol) and *p*-methylbenzylamine (93 mg, 0.77mmol) in toluene (40 mL) was heated under reflux overnight; the water produced was collected in a Dean-Stark apparatus. The solution was allowed to cool to room temperature and the solvent evaporated off under reduced pressure to give 1,3,5-tris[(4-tolyliminomethyl)phenyl]benzene as an off-white solid (170 mg, 95%). ^{1}H NMR (200 MHz, $CDCl_3$): δ = 2.36 (s, 9H), 4.84 (s, 6H), 7.16-7.30 (m, 12H), 7.76 (d, J = 8 Hz, 6H), 7.86 (d, J = 8 Hz, 6H), 7.93 (s, 3H), 8.45 (s, 6H). This solid was dissolved in distilled THF (5 mL) and distilled MeOH (5 mL). $NaBH_4$ (160 mg, 4.2 mmol) was added portionwise and the reaction mixture was left to stir overnight. The reaction mixture was then treated with 5N $HCl_{(aq)}$ until the pH < 1. The solution was concentrated in vacuo, and the residue was partitioned between 2N $NaOH_{(aq)}$ (40 mL) and CH_2Cl_2 (40 mL). The aqueous layer was then extracted further with CH_2Cl_2 (30 mL). The combined organic extracts were washed with H_2O (30 mL) and then dried ($MgSO_4$). Filtration and solvent evaporation gave 1,3,5-tris[(4-tolylaminomethyl)-phenyl]benzene (134 mg, 79 %) as a clear oil. ^{1}H NMR (200 MHz, $CDCl_3$): δ = 2.35 (s, 9H), 3.82 (s, 6H), 3.86 (s, 6H), 7.15 (d, J = 8 Hz, 6H), 7.27 (d, J = 8 Hz, 6H), 7.45 (d, J = 8 Hz, 6H), 7. 65 (d, J = 8 Hz, 6H), 7.74 (s, 3H). This oil was refluxed in 12N $HCl_{(aq)}$ overnight. After cooling, the reaction mixture was filtered and the residue washed with H_2O (20 mL) and CD_3COCD_3 (5 mL). The resulting white solid was dissolved in hot H_2O (80 mL) and saturated $NH_4PF_{6(aq)}$ solution was added. The resulting suspension was extracted with CH_3NO_2 (2 x 50 mL). The combined extracts were washed with H_2O (2 x 100 mL), dried ($MgSO_4$), filtered and solvent removed under reduced pressure to give the trisammonium salt **3**·3PF_6 as an off-white solid (187 mg, 86%). ^{1}H NMR (400 MHz, CD_3CN): δ = 2.36 (s, 9H), 4.23 (m, 6H), 4.29 (m,

6H), 7.12 (br s, 6H), 7.28 (d, J = 8 Hz, 6H), 7.36 (d, J = 8 Hz, 6H), 7.57 (d, J = 8 Hz, 6H), 7.89 (d, J = 8 Hz, 6H), 7.95 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ = 20.3, 51.0, 51.4, 125.3, 125.3, 127.9, 129.7, 130.0, 130.2, 130.8, 140.1, 141.5, 141.6; MS (FAB): *m/z* = 852 [$(M\text{-}PF_6\text{-}HPF_6)^+$].



Experimental Procedure for CD_3SOCD_3 Additions. A 7.5 mM solution of **1** and **3**·3PF_6 in 1:1 v/v $CDCl_3/CD_3CN$ (500 μL) was prepared and successive 10 μL aliquots of CD_3SOCD_3 were added to this solution. After each addition an ^{1}H NMR spectrum was recorded. The chemical shifts reported are referenced to the residual solvent peak of CD_3CN assigned as 1.94 ppm.

References

(1) (a) Beattie, D. R.; Hindmarsh, P.; Goodby, J. W.; Haslam, S. D.; Richardson, R. M. *J. Mater. Chem.* **1992**, *2*, 1261-1266. (b) Boden, N.; Borner, R. C.; Bushby, R. J.; Cammidge, A. N.; Jesudason, M. V. *Liquid Crystals* **1993**, *15*, 851-858.

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Table 1. Crystal data and structure refinement for $[\mathbf{1}\cdot\mathbf{2}]^{3+}$

Identification code	FS9904
Empirical formula	$C_{138.50}H_{138}F_{18}N_3O_{24}P_3$
Formula weight	2663.43
Temperature	173(2) K
Diffractometer Used	Siemens P4/RA
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 58.624(2) Å alpha = 90° b = 26.4490(14) Å beta = 107.077(4)° c = 19.2873(9) Å gamma = 90°
Volume, Z	28587(2) Å^3, 8
Density (calculated)	1.238 Mg/m^3
Absorption coefficient	1.146 mm^{-1}
F(000)	11112
Crystal colour/morphology	Clear block
Crystal size	0.33 x 0.67 x 0.85 mm
θ range for data collection	1.58 to 60.00°
Limiting indices	$-44 \le h \le 48$, $-29 \le k \le 2$, $-21 \le l \le 21$
Scan type	ω-scans
Reflections collected	19085
Independent reflections	18858 (R_{int} = 0.0443)
Observed reflections [F>4σ(F)]	8533
Absorption correction	None
Structure solution method	Direct
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	15364 / 2691 / 1925
Goodness-of-fit on F^2	1.832
Final R indices [F>4σ(F)]	R1 = 0.1421, wR2 = 0.3302
R indices (all data)	R1 = 0.2386, wR2 = 0.4026
Largest diff. peak and hole	0.477 and -0.441 eÅ^{-3}
Mean and maximum shift/error	0.082 and -0.601

Table 2. Atomic coordinates [x 10^4], equivalent isotropic displacement parameters [$Å^2$ x 10^3] and site occupancy factors for $[\mathbf{1}\cdot\mathbf{2}]^{3+}$ U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	sof
P(1)	1792(2)	5945(4)	409(5)	138(5)	0.605(11)
F(11)	1555(3)	6201(7)	-85(8)	229(12)	0.605(11)
F(12)	1694(2)	5423(3)	40(6)	129(5)	0.605(11)
F(13)	1912(3)	6043(5)	-235(5)	155(6)	0.605(11)
F(14)	1883(4)	6466(5)	764(9)	200(9)	0.605(11)
F(15)	1683(2)	5832(6)	1053(6)	159(6)	0.605(11)
F(16)	2030(2)	5669(4)	858(5)	113(4)	0.605(11)
P(1')	1762(3)	6048(6)	319(8)	135(7)	0.395(11)
F(11')	1745(4)	6526(8)	-112(13)	177(10)	0.395(11)
F(12')	1777(3)	6350(8)	1002(9)	131(9)	0.395(11)
F(13')	2032(3)	6024(8)	509(13)	183(10)	0.395(11)
F(14')	1734(5)	5742(10)	-355(13)	249(14)	0.395(11)
F(15')	1486(3)	6037(7)	174(10)	114(7)	0.395(11)
F(16')	1774(4)	5564(8)	766(13)	189(10)	0.395(11)
P(2)	2854(1)	2896(2)	2802(3)	163(2)	1
F(21)	2918(2)	3088(5)	2109(6)	264(7)	1
F(22)	3022(2)	2442(3)	2793(6)	229(5)	1
F(23)	2637(2)	2609(4)	2283(5)	229(5)	1
F(24)	2695(2)	3360(5)	2780(10)	391(13)	1
F(25)	3073(2)	3184(5)	3297(6)	275(8)	1
F(26)	2802(3)	2675(7)	3474(7)	407(13)	1
P(3)	0	2993(2)	7500	122(2)	1
F(31)	13(2)	3019(4)	6699(4)	219(5)	1
F(32)	0	3604(4)	7500	198(6)	1
F(33)	276(1)	3021(4)	7812(5)	198(4)	1
F(34)	0	2417(4)	7500	313(14)	1
P(4)	-315(3)	8697(6)	-681(8)	298(11)	0.50
F(41)	-84(4)	8972(10)	-693(16)	349(18)	0.50
F(42)	-313(5)	8968(10)	33(12)	305(16)	0.50
F(43)	-163(4)	8270(8)	-224(13)	266(12)	0.50
F(44)	-314(6)	8426(12)	-1390(12)	455(28)	0.50
F(45)	-468(6)	9120(11)	-1134(18)	531(34)	0.50
F(46)	-543(4)	8417(12)	-656(16)	365(20)	0.50
O(1)	764(1)	7337(3)	1367(3)	99(2)	1
C(2)	554(2)	7380(5)	1586(7)	124(4)	1
C(3)	371(2)	7673(5)	1041(8)	151(6)	1
O(4)	440(2)	8181(4)	1034(6)	148(4)	1
C(5)	336(7)	8516(6)	1409(22)	179(19)	0.50
C(5A)	272(4)	8547(7)	931(27)	201(23)	0.50
C(6)	329(3)	9031(6)	1141(17)	281(15)	1
O(7)	547(2)	9254(5)	1313(12)	278(9)	1
C(8)	559(3)	9788(6)	1202(16)	299(17)	1
C(9)	774(4)	10017(7)	1624(14)	243(12)	1
O(10)	974(3)	9860(4)	1482(8)	199(6)	1
C(11)	1194(3)	10086(5)	1783(9)	159(6)	1
C(12)	1226(4)	10378(6)	2400(10)	320(20)	1
C(13)	1456(4)	10571(6)	2623(12)	324(22)	1
C(14)	1643(3)	10517(5)	2326(10)	210(11)	1
C(15)	1589(3)	10216(5)	1712(9)	207(10)	1
C(16)	1363(3)	10010(4)	1460(7)	148(6)	1
O(17)	1284(2)	9711(4)	868(6)	185(5)	1
C(18)	1441(4)	9708(7)	407(10)	256(13)	1
C(19)	1320(5)	9463(6)	-259(9)	269(14)	1

O(20)	1303(4)	8939(5)	-188(9)	296(11)	1
C(21)	1421(4)	8626(6)	-508(14)	202(9)	1
C(22)	1421(5)	8115(6)	-451(14)	286(15)	1
O(23)	1288(2)	7885(4)	-59(5)	165(4)	1
C(24)	1287(4)	7338(5)	-116(8)	202(9)	1
C(25)	1328(2)	7109(5)	585(6)	140(5)	1
O(26)	1135(1)	7234(3)	896(3)	105(2)	1
C(27)	1148(2)	6997(3)	1550(4)	83(3)	1
C(28)	1351(2)	6743(4)	1950(5)	89(3)	1
C(29)	1347(2)	6507(3)	2616(4)	70(2)	1
C(30)	1558(2)	6244(3)	3063(4)	67(2)	1
C(31)	1774(2)	6241(4)	2888(5)	81(3)	1
C(32)	1972(2)	6012(3)	3305(5)	77(2)	1
O(33)	2190(1)	5986(3)	3183(3)	95(2)	1
C(34)	2203(2)	6144(4)	2500(6)	108(3)	1
C(35)	2432(2)	5963(6)	2394(7)	140(5)	1
O(36)	2635(2)	6201(4)	2893(5)	130(3)	1
C(37)	2727(3)	6577(5)	2551(6)	170(7)	1
C(38)	2895(2)	6904(5)	3112(9)	167(7)	1
O(39)	3098(2)	6630(3)	3454(4)	118(3)	1
C(40)	3282(2)	6931(5)	3901(6)	139(5)	1
C(41)	3496(2)	6629(5)	4210(7)	140(5)	1
O(42)	3466(2)	6333(4)	4788(5)	137(3)	1
C(43)	3668(3)	6087(5)	5200(7)	151(6)	1
C(44)	3874(3)	6033(8)	4995(11)	190(8)	1
C(45)	4066(4)	5788(9)	5469(13)	219(11)	1
C(46)	4060(3)	5588(9)	6127(14)	224(10)	1
C(47)	3847(3)	5634(7)	6291(8)	164(6)	1
C(48)	3654(3)	5888(5)	5837(8)	135(5)	1
O(49)	3443(2)	5939(3)	5998(4)	114(2)	1
C(50)	3441(2)	5776(5)	6706(6)	116(4)	1
C(51)	3220(2)	5923(5)	6837(5)	111(4)	1
O(52)	3029(1)	5619(3)	6406(4)	118(2)	1
C(53)	2844(2)	5562(5)	6711(5)	122(4)	1
C(54)	2677(2)	5178(5)	6316(6)	151(6)	1
O(55)	2573(1)	5301(2)	5594(3)	94(2)	1
C(56)	2398(2)	4945(4)	5197(6)	109(4)	1
C(57)	2162(2)	5191(4)	4910(5)	99(3)	1
O(58)	2176(1)	5526(2)	4349(3)	85(2)	1
C(59)	1967(2)	5750(3)	3948(5)	76(2)	1
C(60)	1760(2)	5733(3)	4123(4)	79(3)	1
C(61)	1549(2)	5976(3)	3684(4)	70(2)	1
C(62)	1324(2)	5944(3)	3856(4)	73(2)	1
C(63)	1288(2)	5634(3)	4416(4)	72(2)	1
C(64)	1086(2)	5602(3)	4580(4)	79(3)	1
O(65)	1046(1)	5295(2)	5109(3)	91(2)	1
C(66)	1229(2)	4958(4)	5456(6)	111(4)	1
C(67)	1159(3)	4669(4)	6027(6)	135(5)	1
O(68)	1140(2)	4999(3)	6572(4)	118(3)	1
C(69)	1218(4)	4839(5)	7262(6)	209(8)	1
C(70)	1253(3)	5196(5)	7848(7)	198(8)	1
O(71)	1341(3)	5646(4)	7687(7)	121(5)	0.50
C(72)	1432(5)	5943(6)	8319(10)	147(9)	0.50
C(73)	1448(4)	6477(7)	8152(15)	173(11)	0.50
O(71A)	1055(4)	5549(7)	7768(8)	189(9)	0.50
C(72A)	1079(6)	5873(6)	8350(12)	202(13)	0.50
C(73A)	1231(7)	6303(9)	8447(12)	197(11)	0.50
O(74)	1197(3)	6691(4)	7914(5)	208(6)	1
C(75)	1221(3)	7180(4)	7742(4)	184(7)	1
C(76)	1445(2)	7399(5)	7882(7)	279(12)	1
C(77)	1453(3)	7901(5)	7685(7)	235(11)	1
C(78)	1242(3)	8156(6)	7369(7)	268(12)	1

C(79)	1018(3)	7941(4)	7229(7)	266(11)	1
C(80)	1018(3)	7438(4)	7429(6)	199(8)	1
O(81)	818(3)	7175(6)	7331(8)	290(9)	1
C(82)	595(4)	7398(9)	7216(15)	333(14)	1
C(83)	390(4)	7054(15)	7042(16)	291(19)	0.50
O(84)	359(5)	6748(11)	6433(13)	262(13)	0.50
C(83A)	493(6)	7531(11)	6462(17)	226(15)	0.50
O(84A)	432(5)	7179(11)	5905(18)	226(11)	0.50
C(85)	212(4)	6933(9)	5781(13)	287(12)	1
C(86)	163(4)	6630(10)	5131(12)	300(13)	1
O(87)	327(2)	6298(5)	5034(7)	185(5)	1
C(88)	285(2)	6059(6)	4358(6)	162(6)	1
C(89)	485(2)	6178(5)	4038(7)	141(5)	1
O(90)	691(1)	5871(3)	4438(4)	116(3)	1
C(91)	890(2)	5920(3)	4205(5)	87(3)	1
C(92)	915(2)	6211(4)	3648(5)	92(3)	1
C(93)	1126(2)	6243(3)	3461(4)	75(2)	1
C(94)	1142(2)	6519(3)	2827(4)	73(2)	1
C(95)	944(2)	6810(3)	2424(4)	81(2)	1
C(96)	950(2)	7047(3)	1790(5)	82(2)	1
C(97)	1474(2)	7632(3)	3746(4)	77(2)	1
C(98)	1715(2)	7540(3)	3951(5)	82(3)	1
C(99)	1824(2)	7217(3)	4533(4)	76(2)	1
C(100)	1688(2)	7028(3)	4927(4)	74(2)	1
C(101)	1448(2)	7131(3)	4776(4)	79(3)	1
C(102)	1340(2)	7433(3)	4156(5)	82(3)	1
C(103)	1363(2)	7929(4)	3069(5)	88(3)	1
C(104)	1149(2)	8159(4)	2974(5)	105(4)	1
C(105)	1029(2)	8417(4)	2298(6)	103(3)	1
C(106)	1137(2)	8428(4)	1776(5)	101(3)	1
C(107)	1362(2)	8212(4)	1877(6)	106(3)	1
C(108)	1470(2)	7956(4)	2519(5)	92(3)	1
C(109)	1010(3)	8664(4)	1038(6)	133(5)	1
N(110)	871(2)	8273(3)	559(4)	96(2)	1
C(111)	736(3)	8426(6)	-190(7)	174(7)	1
C(112)	580(3)	8029(6)	-642(7)	212(9)	1
C(113)	345(3)	8155(6)	-1002(8)	237(9)	1
C(114)	197(2)	7807(8)	-1461(8)	258(11)	1
C(115)	284(4)	7332(7)	-1559(10)	369(17)	1
C(116)	520(4)	7206(6)	-1199(12)	467(20)	1
C(117)	667(3)	7554(7)	-740(10)	429(18)	1
C(118)	2075(2)	7081(3)	4682(4)	77(2)	1
C(119)	2179(2)	7075(3)	4130(5)	86(3)	1
C(120)	2407(2)	6911(3)	4242(5)	89(3)	1
C(121)	2545(2)	6726(3)	4904(5)	82(3)	1
C(122)	2447(2)	6747(4)	5467(5)	93(3)	1
C(123)	2222(2)	6915(3)	5363(4)	87(3)	1
C(124)	2781(2)	6502(4)	4988(6)	106(3)	1
N(125)	2743(2)	5956(3)	4678(5)	105(3)	1
C(126)	2960(2)	5725(4)	4594(6)	118(4)	1
C(127)	2934(2)	5168(2)	4460(4)	116(4)	1
C(128)	3007(2)	4836(3)	5042(4)	133(4)	1
C(129)	2979(2)	4318(3)	4926(5)	181(6)	1
C(130)	2878(2)	4132(3)	4229(6)	190(7)	1
C(131)	2804(2)	4464(4)	3648(4)	174(7)	1
C(132)	2832(2)	4982(4)	3763(4)	165(6)	1
C(133)	1297(2)	6935(3)	5213(4)	82(3)	1
C(134)	1379(2)	6545(4)	5712(5)	102(3)	1
C(135)	1242(2)	6334(4)	6104(5)	97(3)	1
C(136)	1018(2)	6492(4)	6001(5)	100(3)	1
C(137)	939(3)	6899(5)	5544(8)	144(5)	1
C(138)	1077(3)	7112(5)	5160(7)	128(4)	1

C(139)	858(2)	6250(5)	6399(7)	119(4)	1
N(140)	769(2)	5744(4)	6065(5)	110(3)	1
C(141)	584(3)	5494(6)	6363(9)	176(7)	1
C(142)	532(3)	4990(4)	6161(8)	152(11)	0.661(13)
C(143)	519(3)	4829(5)	5464(8)	174(11)	0.661(13)
C(144)	483(4)	4321(6)	5282(8)	210(13)	0.661(13)
C(145)	460(4)	3973(5)	5798(10)	214(15)	0.661(13)
C(146)	473(3)	4133(5)	6494(10)	181(10)	0.661(13)
C(147)	509(3)	4642(6)	6676(8)	174(9)	0.661(13)
C(14A)	489(6)	4979(14)	6036(17)	151(22)	0.339(13)
C(14B)	273(6)	5024(12)	5496(18)	134(14)	0.339(13)
C(14C)	169(6)	4601(16)	5099(16)	186(21)	0.339(13)
C(14D)	282(8)	4134(13)	5242(24)	236(32)	0.339(13)
C(14E)	499(8)	4090(12)	5781(27)	346(69)	0.339(13)
C(14F)	602(5)	4512(17)	6178(20)	174(20)	0.339(13)
C(150)	2469(8)	3395(21)	5318(20)	226(26)	0.50
C(151)	2685(14)	3591(28)	5724(29)	348(41)	0.50
C(152)	3049(8)	3120(27)	5839(24)	250(27)	0.50
C(153)	2931(9)	2672(21)	5956(24)	224(21)	0.50
C(154)	2990(11)	2498(24)	5131(37)	415(51)	0.50
C(155)	-662(4)	7750(10)	1420(10)	202(10)	1
C(156)	-397(8)	8394(17)	1563(25)	191(16)	0.50
C(157)	-488(12)	7998(27)	668(24)	270(33)	0.50
C(158)	-533(8)	8225(12)	1859(24)	173(15)	0.50
C(159)	-492(10)	7990(14)	1123(23)	173(17)	0.50
C(160)	-204(11)	9958(28)	6195(34)	278(30)	0.50
C(161)	-179(13)	9707(34)	5502(49)	368(44)	0.50
C(162)	-441(10)	9764(17)	5597(29)	247(23)	0.50
C(163)	-713(7)	8938(19)	6904(16)	209(18)	0.50
C(164)	-502(6)	9080(7)	7369(11)	193(12)	0.70
C(165)	-582(14)	9319(29)	6739(41)	202(28)	0.30
C(166)	-72(21)	10620(32)	7186(48)	276(44)	0.30
C(167)	-285(16)	10412(38)	5998(52)	258(37)	0.30
C(168)	-313(15)	10482(30)	7007(44)	236(31)	0.30
C(169)	31(10)	5602(29)	8258(20)	243(26)	0.50
C(170)	328(9)	5430(13)	7789(25)	205(18)	0.50
C(171)	123(9)	5764(16)	7586(27)	210(26)	0.50
C(172)	101(17)	5791(35)	7018(64)	202(34)	0.30
C(173)	24(17)	5159(26)	7806(39)	202(30)	0.30
C(174)	117(15)	6142(33)	7714(57)	246(41)	0.30
C(175)	2132(6)	3932(17)	3310(23)	239(18)	0.70
C(176)	2012(8)	4227(7)	2437(18)	166(17)	0.50
C(177)	1979(4)	3409(9)	2192(12)	219(9)	1
C(178)	1857(10)	4708(24)	2293(42)	273(26)	0.50
C(179)	2092(13)	4451(28)	3094(33)	289(33)	0.50
C(180)	1829(7)	3982(27)	2139(29)	293(32)	0.50
C(181)	2228(6)	4293(23)	2062(24)	228(23)	0.50
C(182)	1944(11)	4529(20)	1671(29)	253(26)	0.50
C(183)	2059(12)	3975(18)	2397(26)	235(26)	0.50
C(184)	797(16)	5515(20)	8525(22)	395(50)	0.50
C(185)	896(8)	6225(13)	9530(19)	198(17)	0.50
C(186)	789(12)	5863(22)	8803(34)	290(30)	0.50

Table 3. Bond Lengths [Å] and angles [°] for $[\mathbf{1}\cdot\mathbf{2}]^{3+}$

P(1)-F(14)	1.562(13)	P(1)-F(11)	1.59(2)
P(1)-F(12)	1.581(10)	P(1)-F(16)	1.589(14)
P(1)-F(15)	1.585(14)	P(1)-F(13)	1.618(13)
P(1')-F(11')	1.50(2)	P(1')-F(14')	1.50(2)
P(1')-F(16')	1.53(2)	P(1')-F(13')	1.52(2)
P(1')-F(12')	1.52(2)	P(1')-F(15')	1.56(2)
P(2)-F(26)	1.533(12)	P(2)-F(24)	1.533(10)
P(2)-F(25)	1.556(9)	P(2)-F(22)	1.558(10)
P(2)-F(23)	1.566(9)	P(2)-F(21)	1.576(11)
P(3)-F(34)	1.524(12)	P(3)-F(33)	1.551(8)
P(3)-F(33)#1	1.551(8)	P(3)-F(31)#1	1.570(8)
P(3)-F(31)	1.570(8)	P(3)-F(32)	1.617(12)
P(4)-F(45)	1.536(10)	P(4)-F(46)	1.543(11)
P(4)-F(41)	1.545(11)	P(4)-F(43)	1.544(10)
P(4)-F(44)	1.547(10)	P(4)-F(42)	1.549(10)
O(1)-C(96)	1.385(10)	O(1)-C(2)	1.418(12)
C(2)-C(3)	1.482(13)	C(3)-O(4)	1.404(12)
O(4)-C(5A)	1.35(2)	O(4)-C(5)	1.39(2)
C(5)-C(6)	1.45(2)	C(5A)-C(6)	1.35(2)
C(6)-O(7)	1.36(2)	O(7)-C(8)	1.43(2)
C(8)-C(9)	1.42(2)	C(9)-O(10)	1.35(2)
O(10)-C(11)	1.38(2)	C(11)-C(16)	1.33(2)
C(11)-C(12)	1.385(2)	C(12)-C(13)	1.385(2)
C(13)-C(14)	1.385(2)	C(14)-C(15)	1.385(2)
C(15)-C(16)	1.385(2)	C(16)-O(17)	1.353(14)
O(17)-C(18)	1.45(2)	C(18)-C(19)	1.43(2)
C(19)-O(20)	1.40(2)	O(20)-C(21)	1.34(2)
C(21)-C(22)	1.36(2)	C(22)-O(23)	1.379(14)
O(23)-C(24)	1.452(13)	C(24)-C(25)	1.435(13)
C(25)-O(26)	1.468(11)	O(26)-C(27)	1.390(10)
C(27)-C(96)	1.375(13)	C(27)-C(28)	1.390(13)
C(28)-C(29)	1.434(12)	C(29)-C(94)	1.380(13)
C(29)-C(30)	1.460(12)	C(30)-C(31)	1.404(13)
C(30)-C(61)	1.407(11)	C(31)-C(32)	1.344(12)
C(32)-O(33)	1.367(10)	C(32)-C(59)	1.429(13)
O(33)-C(34)	1.405(10)	C(34)-C(35)	1.494(13)
C(35)-O(36)	1.439(11)	O(36)-C(37)	1.388(12)
C(37)-C(38)	1.50(2)	C(38)-O(39)	1.384(12)
O(39)-C(40)	1.414(12)	C(40)-C(41)	1.46(2)
C(41)-O(42)	1.413(12)	O(42)-C(43)	1.380(13)
C(43)-C(48)	1.36(2)	C(43)-C(44)	1.385(2)
C(44)-C(45)	1.385(2)	C(45)-C(46)	1.385(2)
C(46)-C(47)	1.384(2)	C(47)-C(48)	1.385(2)
C(48)-O(49)	1.364(13)	O(49)-C(50)	1.436(11)
C(50)-C(51)	1.445(13)	C(51)-O(52)	1.429(10)
O(52)-C(53)	1.385(11)	C(53)-C(54)	1.459(13)
C(54)-O(55)	1.385(11)	O(55)-C(56)	1.436(11)
C(56)-C(57)	1.482(12)	C(57)-O(58)	1.420(9)
O(58)-C(59)	1.378(9)	C(59)-C(60)	1.348(13)
C(60)-C(61)	1.432(12)	C(61)-C(62)	1.453(12)
C(62)-C(93)	1.425(12)	C(62)-C(63)	1.420(12)
C(63)-C(64)	1.317(12)	C(64)-O(65)	1.376(9)
C(64)-C(91)	1.435(12)	O(65)-C(66)	1.404(10)
C(66)-C(67)	1.494(12)	C(67)-O(68)	1.396(11)
O(68)-C(69)	1.344(11)	C(69)-C(70)	1.44(2)
C(70)-O(71)	1.37(2)	C(70)-O(71A)	1.46(2)
O(71)-C(72)	1.42(2)	C(72)-C(73)	1.46(2)
C(73)-O(74)	1.51(2)	O(71A)-C(72A)	1.39(2)
C(72A)-C(73A)	1.42(2)	C(73A)-O(74)	1.42(2)

O(74)-C(75)	1.353(12)	C(75)-C(80)	1.35(2)
C(75)-C(76)	1.3848(11)	C(76)-C(77)	1.3849(11)
C(77)-C(78)	1.3848(11)	C(78)-C(79)	1.3849(11)
C(79)-C(80)	1.3846(11)	C(80)-O(81)	1.328(14)
O(81)-C(82)	1.40(2)	C(82)-C(83A)	1.44(2)
C(82)-C(83)	1.46(2)	C(83)-O(84)	1.39(2)
O(84)-C(85)	1.39(2)	C(83A)-O(84A)	1.39(2)
O(84A)-C(85)	1.40(2)	C(85)-C(86)	1.44(2)
C(86)-O(87)	1.36(2)	O(87)-C(88)	1.405(14)
C(88)-C(89)	1.505(14)	C(89)-O(90)	1.473(11)
O(90)-C(91)	1.375(10)	C(91)-C(92)	1.364(13)
C(92)-C(93)	1.388(13)	C(93)-C(94)	1.450(12)
C(94)-C(95)	1.417(12)	C(95)-C(96)	1.383(12)
C(97)-C(102)	1.373(13)	C(97)-C(98)	1.372(13)
C(97)-C(103)	1.498(12)	C(98)-C(99)	1.405(12)
C(99)-C(100)	1.347(12)	C(99)-C(118)	1.462(13)
C(100)-C(101)	1.377(13)	C(101)-C(102)	1.423(11)
C(101)-C(133)	1.484(13)	C(103)-C(104)	1.36(2)
C(103)-C(108)	1.384(14)	C(104)-C(105)	1.456(13)
C(105)-C(106)	1.34(2)	C(106)-C(107)	1.40(2)
C(106)-C(109)	1.532(13)	C(107)-C(108)	1.390(13)
C(109)-N(110)	1.464(13)	N(110)-C(111)	1.484(13)
C(111)-C(112)	1.49(2)	C(112)-C(113)	1.39
C(112)-C(117)	1.39	C(113)-C(114)	1.39
C(114)-C(115)	1.39	C(115)-C(116)	1.39
C(116)-C(117)	1.39	C(118)-C(119)	1.374(12)
C(118)-C(123)	1.412(12)	C(119)-C(120)	1.362(13)
C(120)-C(121)	1.386(12)	C(121)-C(122)	1.371(13)
C(121)-C(124)	1.465(14)	C(122)-C(123)	1.353(13)
C(124)-N(125)	1.555(13)	N(125)-C(126)	1.459(14)
C(126)-C(127)	1.495(12)	C(127)-C(128)	1.39
C(127)-C(132)	1.39	C(128)-C(129)	1.39
C(129)-C(130)	1.39	C(130)-C(131)	1.39
C(131)-C(132)	1.39	C(133)-C(138)	1.35(2)
C(133)-C(134)	1.396(12)	C(134)-C(135)	1.369(14)
C(135)-C(136)	1.339(14)	C(136)-C(137)	1.383(14)
C(136)-C(139)	1.51(2)	C(137)-C(138)	1.37(2)
C(139)-N(140)	1.511(14)	N(140)-C(141)	1.521(14)
C(141)-C(142)	1.40(2)	C(141)-C(14A)	1.53(3)
C(142)-C(143)	1.39	C(142)-C(147)	1.39
C(143)-C(144)	1.39	C(144)-C(145)	1.39
C(145)-C(146)	1.39	C(146)-C(147)	1.39
C(14A)-C(14B)	1.39	C(14A)-C(14F)	1.39
C(14B)-C(14C)	1.39	C(14C)-C(14D)	1.39
C(14D)-C(14E)	1.39	C(14E)-C(14F)	1.39

F(14)-P(1)-F(11)	90.7(9)	F(14)-P(1)-F(12)	178.7(11)
F(11)-P(1)-F(12)	87.9(8)	F(14)-P(1)-F(16)	91.9(8)
F(11)-P(1)-F(16)	176.2(8)	F(12)-P(1)-F(16)	89.4(7)
F(14)-P(1)-F(15)	89.3(8)	F(11)-P(1)-F(15)	93.9(10)
F(12)-P(1)-F(15)	90.6(8)	F(16)-P(1)-F(15)	88.8(8)
F(14)-P(1)-F(13)	91.4(9)	F(11)-P(1)-F(13)	88.3(9)
F(12)-P(1)-F(13)	88.6(6)	F(16)-P(1)-F(13)	88.9(8)
F(15)-P(1)-F(13)	177.7(11)	F(11')-P(1')-F(14')	90.2(12)
F(11')-P(1')-F(16')	178.4(14)	F(14')-P(1')-F(16')	90.7(12)
F(11')-P(1')-F(13')	93.7(12)	F(14')-P(1')-F(13')	91.6(12)
F(16')-P(1')-F(13')	87.6(12)	F(11')-P(1')-F(12')	90.9(12)
F(14')-P(1')-F(12')	177(2)	F(16')-P(1')-F(12')	88.2(11)
F(13')-P(1')-F(12')	91.2(12)	F(11')-P(1')-F(15')	91.2(11)
F(14')-P(1')-F(15')	89.4(12)	F(16')-P(1')-F(15')	87.5(11)
F(13')-P(1')-F(15')	175.0(14)	F(12')-P(1')-F(15')	87.6(10)
F(26)-P(2)-F(24)	93.3(8)	F(26)-P(2)-F(25)	90.1(7)

F(24)-P(2)-F(25)	90.7(6)	F(26)-P(2)-F(22)	89.9(8)
F(24)-P(2)-F(22)	176.6(9)	F(25)-P(2)-F(22)	88.4(6)
F(26)-P(2)-F(23)	91.6(8)	F(24)-P(2)-F(23)	89.8(7)
F(25)-P(2)-F(23)	178.2(7)	F(22)-P(2)-F(23)	91.0(6)
F(26)-P(2)-F(21)	175.8(9)	F(24)-P(2)-F(21)	90.8(8)
F(25)-P(2)-F(21)	90.2(7)	F(22)-P(2)-F(21)	85.9(7)
F(23)-P(2)-F(21)	88.1(6)	F(34)-P(3)-F(33)	92.7(4)
F(34)-P(3)-F(33)#1	92.7(4)	F(33)-P(3)-F(33)#1	174.5(8)
F(34)-P(3)-F(31)#1	92.5(5)	F(33)-P(3)-F(31)#1	87.8(5)
F(33)#1-P(3)-F(31)#1	92.0(5)	F(34)-P(3)-F(31)	92.5(5)
F(33)-P(3)-F(31)	92.0(5)	F(33)#1-P(3)-F(31)	87.8(5)
F(31)#1-P(3)-F(31)	174.9(9)	F(34)-P(3)-F(32)	180.000(3)
F(33)-P(3)-F(32)	87.3(4)	F(33)#1-P(3)-F(32)	87.3(4)
F(31)#1-P(3)-F(32)	87.5(5)	F(31)-P(3)-F(32)	87.5(5)
F(45)-P(4)-F(46)	90.0(11)	F(45)-P(4)-F(41)	91.0(11)
F(46)-P(4)-F(41)	179.0(12)	F(45)-P(4)-F(43)	179.6(14)
F(46)-P(4)-F(43)	89.7(10)	F(41)-P(4)-F(43)	89.3(10)
F(45)-P(4)-F(44)	89.3(11)	F(46)-P(4)-F(44)	91.9(10)
F(41)-P(4)-F(44)	88.4(10)	F(43)-P(4)-F(44)	90.8(11)
F(45)-P(4)-F(42)	91.2(11)	F(46)-P(4)-F(42)	88.6(10)
F(41)-P(4)-F(42)	91.0(10)	F(43)-P(4)-F(42)	88.8(10)
F(44)-P(4)-F(42)	179.3(14)	C(96)-O(1)-C(2)	118.1(7)
O(1)-C(2)-C(3)	110.0(9)	O(4)-C(3)-C(2)	110.9(10)
C(5A)-O(4)-C(3)	119.1(13)	C(5)-O(4)-C(3)	115.6(12)
O(4)-C(5)-C(6)	112(2)	O(4)-C(5A)-C(6)	122(2)
O(7)-C(6)-C(5A)	128(2)	O(7)-C(6)-C(5)	113(2)
C(6)-O(7)-C(8)	118.4(13)	C(9)-C(8)-O(7)	114(2)
O(10)-C(9)-C(8)	116(2)	C(9)-O(10)-C(11)	123(2)
C(16)-C(11)-O(10)	118(2)	C(16)-C(11)-C(12)	124(2)
O(10)-C(11)-C(12)	119(2)	C(11)-C(12)-C(13)	110(2)
C(14)-C(13)-C(12)	130(3)	C(13)-C(14)-C(15)	114(2)
C(16)-C(15)-C(14)	119(2)	C(11)-C(16)-O(17)	112(2)
C(11)-C(16)-C(15)	123(2)	O(17)-C(16)-C(15)	125(2)
C(16)-O(17)-C(18)	113.6(12)	C(19)-C(18)-O(17)	109(2)
O(20)-C(19)-C(18)	113(2)	C(21)-O(20)-C(19)	120(2)
O(20)-C(21)-C(22)	125(2)	C(21)-C(22)-O(23)	119.8(14)
C(22)-O(23)-C(24)	112.9(11)	C(25)-C(24)-O(23)	110.7(12)
C(24)-C(25)-O(26)	110.6(10)	C(27)-O(26)-C(25)	115.2(7)
C(96)-C(27)-C(28)	122.1(8)	C(96)-C(27)-O(26)	115.8(9)
C(28)-C(27)-O(26)	122.1(9)	C(27)-C(28)-C(29)	118.1(9)
C(94)-C(29)-C(28)	120.0(9)	C(94)-C(29)-C(30)	119.9(8)
C(28)-C(29)-C(30)	120.1(9)	C(31)-C(30)-C(61)	117.8(8)
C(31)-C(30)-C(29)	121.9(8)	C(61)-C(30)-C(29)	120.3(9)
C(32)-C(31)-C(30)	122.6(9)	C(31)-C(32)-O(33)	127.2(9)
C(31)-C(32)-C(59)	120.2(9)	O(33)-C(32)-C(59)	112.6(9)
C(32)-O(33)-C(34)	117.2(8)	O(33)-C(34)-C(35)	109.3(9)
O(36)-C(35)-C(34)	111.7(10)	C(37)-O(36)-C(35)	111.0(10)
O(36)-C(37)-C(38)	109.5(10)	O(39)-C(38)-C(37)	109.3(11)
C(38)-O(39)-C(40)	113.1(10)	O(39)-C(40)-C(41)	110.6(11)
O(42)-C(41)-C(40)	109.6(11)	C(43)-O(42)-C(41)	115.7(10)
C(48)-C(43)-O(42)	115.6(14)	C(48)-C(43)-C(44)	121(2)
O(42)-C(43)-C(44)	124(2)	C(45)-C(44)-C(43)	118(2)
C(44)-C(45)-C(46)	123(2)	C(47)-C(46)-C(45)	116(2)
C(46)-C(47)-C(48)	122(2)	C(43)-C(48)-O(49)	118(2)
C(43)-C(48)-C(47)	120(2)	O(49)-C(48)-C(47)	122.0(14)
C(48)-O(49)-C(50)	116.7(10)	O(49)-C(50)-C(51)	110.2(9)
O(52)-C(51)-C(50)	109.6(9)	C(53)-O(52)-C(51)	113.1(8)
O(52)-C(53)-C(54)	110.1(10)	O(55)-C(54)-C(53)	113.0(9)
C(54)-O(55)-C(56)	114.6(7)	O(55)-C(56)-C(57)	110.9(9)
O(58)-C(57)-C(56)	107.6(8)	C(59)-O(58)-C(57)	117.1(7)
C(60)-C(59)-O(58)	124.2(9)	C(60)-C(59)-C(32)	118.9(8)
O(58)-C(59)-C(32)	117.0(9)	C(59)-C(60)-C(61)	121.5(9)

C(30)-C(61)-C(60)	119.0(8)	C(30)-C(61)-C(62)	119.2(8)
C(60)-C(61)-C(62)	121.7(8)	C(93)-C(62)-C(63)	116.7(9)
C(93)-C(62)-C(61)	119.8(8)	C(63)-C(62)-C(61)	123.5(9)
C(64)-C(63)-C(62)	124.3(9)	C(63)-C(64)-O(65)	125.3(8)
C(63)-C(64)-C(91)	118.9(8)	O(65)-C(64)-C(91)	115.8(9)
C(64)-O(65)-C(66)	117.0(8)	O(65)-C(66)-C(67)	109.8(9)
O(68)-C(67)-C(66)	109.6(9)	C(69)-O(68)-C(67)	118.1(8)
O(68)-C(69)-C(70)	120.0(10)	O(71)-C(70)-C(69)	111.6(13)
O(71A)-C(70)-C(69)	114.2(13)	C(70)-O(71)-C(72)	111.0(13)
O(71)-C(72)-C(73)	112(2)	C(72)-C(73)-O(74)	108(2)
C(72A)-O(71A)-C(70)	115(2)	O(71A)-C(72A)-C(73A)	121(2)
O(74)-C(73A)-C(72A)	122(2)	C(75)-O(74)-C(73A)	149.8(11)
C(75)-O(74)-C(73)	105.7(12)	C(80)-C(75)-O(74)	116.9(11)
C(80)-C(75)-C(76)	122.3(11)	O(74)-C(75)-C(76)	120.8(12)
C(75)-C(76)-C(77)	117.0(11)	C(78)-C(77)-C(76)	119.4(12)
C(79)-C(78)-C(77)	124.0(12)	C(80)-C(79)-C(78)	114.5(11)
C(75)-C(80)-O(81)	115.1(11)	C(75)-C(80)-C(79)	122.8(12)
O(81)-C(80)-C(79)	122.2(14)	C(80)-O(81)-C(82)	124(2)
O(81)-C(82)-C(83A)	111(3)	O(81)-C(82)-C(83)	116(2)
O(84)-C(83)-C(82)	117(2)	C(85)-O(84)-C(83)	117(2)
O(84A)-C(83A)-C(82)	124(3)	C(83A)-O(84A)-C(85)	117(2)
O(84)-C(85)-C(86)	120(2)	O(84A)-C(85)-C(86)	110(3)
O(87)-C(86)-C(85)	121(2)	C(86)-O(87)-C(88)	118.8(12)
O(87)-C(88)-C(89)	110.0(12)	O(90)-C(89)-C(88)	106.8(9)
C(91)-O(90)-C(89)	115.1(7)	O(90)-C(91)-C(92)	127.4(9)
O(90)-C(91)-C(64)	114.2(8)	C(92)-C(91)-C(64)	118.3(9)
C(91)-C(92)-C(93)	123.3(9)	C(92)-C(93)-C(62)	118.3(8)
C(92)-C(93)-C(94)	122.2(9)	C(62)-C(93)-C(94)	119.1(9)
C(29)-C(94)-C(95)	119.6(8)	C(29)-C(94)-C(93)	120.9(8)
C(95)-C(94)-C(93)	119.5(9)	C(96)-C(95)-C(94)	120.3(9)
C(95)-C(96)-C(27)	119.6(8)	C(95)-C(96)-O(1)	123.5(9)
C(27)-C(96)-O(1)	116.9(8)	C(102)-C(97)-C(98)	118.7(8)
C(102)-C(97)-C(103)	121.8(10)	C(98)-C(97)-C(103)	119.5(9)
C(97)-C(98)-C(99)	121.7(9)	C(100)-C(99)-C(98)	118.2(9)
C(100)-C(99)-C(118)	121.7(8)	C(98)-C(99)-C(118)	120.1(9)
C(99)-C(100)-C(101)	122.9(8)	C(100)-C(101)-C(102)	117.6(9)
C(100)-C(101)-C(133)	123.7(8)	C(102)-C(101)-C(133)	118.7(10)
C(97)-C(102)-C(101)	120.7(10)	C(104)-C(103)-C(108)	118.9(9)
C(104)-C(103)-C(97)	120.0(10)	C(108)-C(103)-C(97)	121.1(10)
C(103)-C(104)-C(105)	120.8(11)	C(106)-C(105)-C(104)	118.5(11)
C(105)-C(106)-C(107)	121.4(10)	C(105)-C(106)-C(109)	120.0(12)
C(107)-C(106)-C(109)	118.5(11)	C(108)-C(107)-C(106)	119.2(11)
C(103)-C(108)-C(107)	121.2(11)	N(110)-C(109)-C(106)	109.1(8)
C(109)-N(110)-C(111)	117.4(10)	N(110)-C(111)-C(112)	115.8(12)
C(113)-C(112)-C(117)	120.0	C(113)-C(112)-C(111)	118.0(10)
C(117)-C(112)-C(111)	121.9(10)	C(112)-C(113)-C(114)	120.0
C(115)-C(114)-C(113)	120.0	C(114)-C(115)-C(116)	120.0
C(115)-C(116)-C(117)	120.0	C(116)-C(117)-C(112)	120.0
C(119)-C(118)-C(123)	115.5(9)	C(119)-C(118)-C(99)	120.0(8)
C(123)-C(118)-C(99)	124.3(9)	C(120)-C(119)-C(118)	121.3(9)
C(119)-C(120)-C(121)	122.7(10)	C(122)-C(121)-C(120)	116.6(10)
C(122)-C(121)-C(124)	121.9(9)	C(120)-C(121)-C(124)	121.5(10)
C(123)-C(122)-C(121)	121.0(9)	C(122)-C(123)-C(118)	122.8(9)
C(121)-C(124)-N(125)	108.1(9)	C(126)-N(125)-C(124)	113.7(9)
N(125)-C(126)-C(127)	112.6(9)	C(128)-C(127)-C(132)	120.0
C(128)-C(127)-C(126)	119.4(6)	C(132)-C(127)-C(126)	120.6(6)
C(129)-C(128)-C(127)	120.0	C(130)-C(129)-C(128)	120.0
C(131)-C(130)-C(129)	120.0	C(130)-C(131)-C(132)	120.0
C(131)-C(132)-C(127)	120.0	C(138)-C(133)-C(134)	115.9(10)
C(138)-C(133)-C(101)	123.6(9)	C(134)-C(133)-C(101)	120.5(10)
C(135)-C(134)-C(133)	122.9(11)	C(136)-C(135)-C(134)	120.0(9)
C(135)-C(136)-C(137)	117.7(10)	C(135)-C(136)-C(139)	121.3(9)

C(137)-C(136)-C(139)	120.9(12)	C(138)-C(137)-C(136)	121.9(12)
C(133)-C(138)-C(137)	121.3(10)	N(140)-C(139)-C(136)	110.2(9)
C(139)-N(140)-C(141)	114.7(10)	C(142)-C(141)-N(140)	115.5(12)
N(140)-C(141)-C(14A)	116(2)	C(143)-C(142)-C(147)	120.0
C(143)-C(142)-C(141)	120.4(10)	C(147)-C(142)-C(141)	119.5(10)
C(144)-C(143)-C(142)	120.0	C(145)-C(144)-C(143)	120.0
C(144)-C(145)-C(146)	120.0	C(147)-C(146)-C(145)	120.0
C(146)-C(147)-C(142)	120.0	C(14B)-C(14A)-C(14F)	120.0
C(14B)-C(14A)-C(141)	112(3)	C(14F)-C(14A)-C(141)	128(3)
C(14A)-C(14B)-C(14C)	120.0	C(14D)-C(14C)-C(14B)	120.0
C(14C)-C(14D)-C(14E)	120.00(6)	C(14F)-C(14E)-C(14D)	120.0
C(14E)-C(14F)-C(14A)	120.0		

E

Table 4. Anisotropic displacement parameters [Å^2 x 10^3] for [**1**·**2**]$^{3+}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [(ha*)^{2}U$_{11}$ + ... + 2hka*b*U$_{12}$].

	U11	U22	U33	U23	U13	U12
P(1)	190(10)	104(6)	106(5)	-62(5)	21(6)	9(5)
F(11)	309(25)	220(21)	107(11)	-42(13)	-17(15)	119(20)
F(12)	153(10)	97(7)	157(10)	-68(7)	74(8)	-27(6)
F(13)	254(16)	143(10)	87(7)	-25(7)	80(9)	-51(11)
F(14)	330(26)	100(9)	182(16)	-56(10)	94(16)	-31(13)
F(15)	119(10)	221(15)	147(10)	-101(10)	52(8)	-24(9)
F(16)	129(10)	111(7)	100(7)	-18(6)	34(6)	13(7)
P(1')	180(14)	111(8)	134(11)	17(7)	79(10)	58(8)
F(11')	143(19)	182(22)	209(23)	48(19)	59(17)	0(16)
F(12')	121(15)	167(21)	93(11)	-75(13)	14(10)	28(14)
F(13')	153(19)	139(17)	256(28)	29(19)	59(19)	38(16)
P(2)	203(5)	133(3)	155(4)	-35(3)	53(3)	5(3)
F(21)	282(14)	255(14)	216(11)	74(10)	13(10)	-67(11)
F(22)	316(15)	126(6)	239(11)	-15(7)	71(11)	45(8)
F(23)	276(13)	225(10)	183(9)	-59(8)	61(9)	-114(10)
F(24)	275(16)	265(15)	580(32)	-251(19)	40(18)	98(13)
F(25)	174(9)	343(16)	270(13)	-200(13)	4(9)	-15(10)
F(26)	556(33)	522(32)	215(14)	82(17)	225(19)	-20(27)
P(3)	111(4)	152(4)	88(3)	0	8(2)	0
F(31)	237(10)	317(13)	104(5)	13(7)	52(6)	102(10)
F(32)	198(13)	156(10)	218(14)	0	25(11)	0
F(33)	105(6)	249(11)	209(9)	-30(8)	-4(6)	33(6)
F(34)	443(29)	117(9)	231(16)	0	-132(18)	0
P(4)	339(24)	260(19)	230(17)	37(15)	-19(18)	-67(18)
F(41)	524(56)	258(33)	285(33)	-6(28)	150(37)	-43(36)
F(42)	256(28)	322(35)	297(33)	-69(29)	17(27)	78(26)
F(43)	231(25)	275(29)	247(26)	23(23)	-2(20)	39(23)
F(44)	376(45)	465(55)	471(58)	-47(49)	42(45)	-203(43)
F(45)	504(61)	311(43)	623(66)	149(46)	-76(53)	103(43)
F(46)	284(36)	477(54)	320(37)	45(38)	67(32)	-63(37)
O(1)	79(5)	120(5)	87(4)	33(4)	9(4)	5(4)
C(2)	79(8)	147(11)	129(9)	48(8)	5(7)	-5(7)
C(3)	71(8)	184(15)	182(14)	76(11)	11(8)	7(9)
O(4)	114(7)	130(7)	200(10)	61(7)	47(7)	39(6)
C(5)	188(38)	93(21)	296(58)	19(25)	131(36)	-10(23)
C(5A)	172(39)	228(49)	217(46)	41(35)	78(33)	31(36)
C(6)	131(18)	152(17)	577(49)	-5(25)	132(25)	21(15)
O(7)	124(10)	157(12)	514(28)	-6(15)	32(14)	34(9)
C(8)	172(20)	109(13)	552(48)	-65(20)	8(25)	28(13)
C(9)	194(23)	153(17)	348(34)	-13(19)	23(23)	12(18)
O(10)	152(11)	170(11)	282(17)	-13(11)	72(12)	8(10)
C(11)	189(19)	172(16)	127(12)	38(11)	63(14)	27(14)
C(12)	323(38)	423(46)	273(35)	141(33)	178(32)	37(33)
C(13)	627(60)	186(20)	232(23)	104(17)	240(32)	245(30)
C(14)	274(26)	75(9)	233(22)	8(10)	-2(19)	-6(12)
C(15)	180(19)	145(15)	330(30)	-7(17)	127(19)	-43(14)
C(16)	194(18)	157(13)	117(11)	21(9)	85(13)	2(13)
O(17)	249(13)	176(10)	167(10)	14(8)	118(10)	-54(9)
C(18)	438(39)	187(19)	210(21)	-2(16)	199(26)	-87(22)
C(19)	495(43)	168(19)	190(19)	40(15)	174(25)	-63(23)
O(20)	554(33)	123(10)	311(19)	15(11)	280(21)	-42(15)
C(21)	208(20)	125(14)	300(28)	52(16)	116(19)	3(13)
C(22)	432(39)	231(25)	313(29)	31(22)	291(30)	12(26)

O(23)	223(11)	158(8)	162(8)	58(7)	131(8)	40(8)
C(24)	344(26)	152(14)	160(14)	59(11)	154(16)	96(16)
C(25)	190(14)	144(10)	100(8)	44(7)	67(9)	75(10)
O(26)	128(6)	114(5)	79(4)	26(4)	38(4)	26(5)
C(27)	76(7)	99(7)	75(5)	-3(5)	24(5)	2(6)
C(28)	106(8)	90(6)	78(6)	-2(5)	40(6)	-2(6)
C(29)	77(7)	69(5)	67(5)	-5(4)	24(5)	3(4)
C(30)	73(7)	54(4)	71(5)	-3(4)	16(5)	2(4)
C(31)	80(8)	93(6)	67(5)	-10(4)	17(5)	5(6)
C(32)	60(7)	76(5)	97(7)	-18(5)	28(6)	-1(5)
O(33)	102(6)	104(5)	81(4)	1(3)	30(4)	8(4)
C(34)	103(9)	116(8)	112(8)	1(6)	41(7)	26(7)
C(35)	106(11)	200(15)	120(10)	-38(10)	39(8)	-33(10)
O(36)	117(7)	160(8)	131(6)	1(6)	64(6)	8(6)
C(37)	302(23)	117(10)	109(10)	28(8)	90(13)	22(13)
C(38)	193(17)	115(11)	244(20)	27(12)	142(16)	28(12)
O(39)	157(8)	105(5)	101(5)	-19(4)	53(5)	-41(6)
C(40)	200(16)	131(11)	109(9)	-33(8)	83(10)	-66(11)
C(41)	172(15)	150(12)	115(10)	-26(9)	70(10)	-78(11)
O(42)	137(8)	185(9)	97(6)	-30(6)	48(6)	-59(7)
C(43)	141(15)	212(17)	110(11)	-49(11)	53(11)	-48(13)
C(44)	138(15)	263(24)	196(19)	-23(17)	93(16)	-30(16)
C(45)	142(19)	307(31)	224(25)	-43(23)	80(19)	23(19)
C(46)	190(23)	261(26)	243(27)	2(21)	95(20)	59(19)
C(47)	140(14)	209(18)	144(13)	-50(13)	42(12)	10(13)
C(48)	149(15)	133(11)	120(11)	-33(9)	36(11)	-13(10)
O(49)	117(7)	133(6)	101(5)	-31(4)	47(5)	-27(5)
C(50)	112(10)	117(8)	100(8)	-2(6)	2(7)	-17(8)
C(51)	88(8)	147(10)	85(6)	-19(7)	7(6)	-15(8)
O(52)	109(6)	144(7)	99(5)	-17(5)	25(5)	-30(5)
C(53)	118(10)	165(12)	83(7)	4(7)	30(7)	-30(9)
C(54)	146(12)	166(12)	123(10)	38(9)	12(9)	-66(10)
O(55)	76(4)	107(5)	85(4)	28(3)	2(3)	-10(4)
C(56)	80(8)	120(8)	119(8)	36(7)	15(6)	18(7)
C(57)	101(8)	92(7)	94(7)	26(5)	16(6)	-12(6)
O(58)	64(4)	95(4)	94(4)	-3(3)	18(3)	0(3)
C(59)	62(7)	74(5)	88(6)	-4(4)	17(5)	-1(5)
C(60)	72(7)	92(6)	63(5)	-10(4)	5(5)	-10(5)
C(61)	66(7)	80(5)	64(5)	-20(4)	20(5)	-13(5)
C(62)	75(7)	80(5)	55(4)	-24(4)	7(4)	-19(5)
C(63)	68(7)	87(6)	56(4)	-3(4)	13(4)	1(5)
C(64)	90(8)	77(5)	70(5)	13(4)	24(5)	-2(5)
O(65)	86(5)	95(4)	91(4)	28(3)	27(4)	5(4)
C(66)	139(10)	97(7)	108(8)	23(6)	54(7)	30(7)
C(67)	195(14)	119(9)	116(9)	45(8)	86(10)	44(9)
O(68)	143(7)	129(6)	90(5)	51(4)	47(5)	45(5)
C(69)	331(21)	105(9)	130(11)	38(9)	-26(13)	44(12)
C(70)	319(21)	134(12)	114(10)	34(10)	21(13)	11(14)
O(71)	194(16)	74(8)	93(9)	13(7)	41(10)	-4(9)
C(72)	191(22)	154(19)	75(12)	-10(14)	7(14)	31(18)
C(73)	246(27)	154(21)	112(17)	14(17)	41(19)	-44(21)
O(71A)	366(28)	117(13)	84(10)	9(9)	67(15)	43(17)
C(72A)	388(33)	97(16)	107(17)	36(14)	53(22)	-41(21)
C(73A)	329(27)	145(19)	105(15)	50(15)	44(18)	-22(20)
O(74)	364(17)	129(8)	109(7)	8(6)	36(9)	-14(10)
C(75)	311(19)	64(7)	227(15)	-84(8)	156(14)	-90(10)
C(76)	368(26)	168(15)	320(23)	-166(16)	132(20)	-72(18)
C(77)	346(26)	203(19)	206(19)	-100(17)	159(18)	-35(20)
C(78)	452(34)	224(20)	174(16)	0(15)	163(21)	-116(22)
C(79)	466(31)	121(13)	234(19)	-17(13)	139(22)	-47(18)
C(80)	333(24)	94(11)	226(16)	-8(11)	171(17)	23(13)
O(81)	260(18)	201(15)	383(20)	-113(14)	54(16)	54(13)

C(82)	317(27)	254(24)	380(28)	-48(21)	29(25)	152(21)
C(83)	233(33)	272(35)	329(36)	-129(30)	22(31)	44(30)
O(84)	206(22)	291(27)	302(29)	-76(23)	95(21)	51(22)
C(83A)	312(31)	158(24)	213(30)	98(21)	85(26)	158(24)
O(84A)	172(19)	230(25)	279(26)	50(20)	70(20)	94(19)
C(85)	154(18)	340(27)	346(29)	-37(23)	40(21)	93(20)
C(86)	155(17)	348(27)	350(28)	-63(23)	0(19)	118(19)
O(87)	115(8)	273(14)	192(10)	92(11)	84(8)	65(9)
C(88)	83(9)	230(17)	171(13)	83(12)	35(9)	8(10)
C(89)	84(8)	176(12)	156(11)	90(10)	24(8)	23(8)
O(90)	69(5)	162(7)	113(5)	58(5)	19(4)	5(4)
C(91)	60(6)	92(6)	107(7)	17(5)	21(5)	-2(5)
C(92)	74(7)	115(7)	82(6)	30(5)	15(5)	-14(6)
C(93)	65(6)	79(5)	75(5)	2(4)	11(4)	-15(4)
C(94)	76(6)	61(4)	72(5)	2(4)	5(4)	3(4)
C(95)	87(7)	82(5)	75(5)	18(4)	25(5)	5(5)
C(96)	87(7)	72(5)	82(5)	6(4)	15(5)	1(5)
C(97)	94(8)	53(4)	75(5)	17(4)	11(5)	-7(5)
C(98)	97(8)	75(5)	70(5)	-2(4)	18(5)	-18(5)
C(99)	100(8)	56(4)	62(5)	4(4)	11(5)	-1(5)
C(100)	87(8)	64(5)	65(5)	3(4)	12(5)	-1(5)
C(101)	113(9)	50(4)	62(5)	-1(3)	8(5)	-19(5)
C(102)	89(7)	70(5)	76(5)	2(4)	9(5)	-12(5)
C(103)	72(7)	96(6)	86(6)	19(5)	6(5)	-27(6)
C(104)	103(9)	108(7)	90(7)	38(6)	4(6)	-37(7)
C(105)	92(8)	86(6)	115(8)	32(6)	5(7)	-10(6)
C(106)	122(10)	95(7)	81(6)	25(5)	23(7)	-31(7)
C(107)	100(9)	117(8)	94(7)	19(6)	17(6)	-13(7)
C(108)	97(7)	104(6)	68(5)	19(5)	12(5)	-16(6)
C(109)	170(12)	108(8)	97(7)	37(6)	2(8)	-31(8)
N(110)	93(6)	113(6)	78(5)	26(4)	18(4)	17(5)
C(111)	172(14)	218(16)	102(9)	47(10)	-6(9)	30(13)
C(112)	180(16)	314(22)	110(10)	-46(13)	-5(10)	99(16)
C(113)	212(20)	297(25)	218(21)	19(19)	87(17)	26(19)
C(114)	242(22)	312(29)	209(20)	-70(20)	49(17)	-39(21)
C(115)	386(32)	357(31)	265(24)	-146(24)	-57(23)	66(27)
C(116)	389(32)	428(33)	386(30)	-195(26)	-192(25)	85(28)
C(117)	377(30)	422(33)	331(28)	-164(25)	-139(24)	120(27)
C(118)	89(8)	71(5)	70(5)	-1(4)	21(5)	4(5)
C(119)	94(8)	80(5)	79(6)	16(4)	18(6)	3(5)
C(120)	114(9)	80(6)	71(5)	8(4)	24(5)	-7(6)
C(121)	92(7)	71(5)	76(6)	5(4)	17(5)	-1(5)
C(122)	99(8)	107(7)	62(5)	-6(5)	7(5)	11(6)
C(123)	106(8)	95(6)	56(5)	-3(4)	19(5)	6(6)
C(124)	134(11)	89(6)	97(7)	6(5)	35(7)	2(7)
N(125)	110(7)	93(5)	125(7)	24(5)	55(6)	19(5)
C(126)	122(10)	118(9)	120(8)	22(7)	46(7)	-13(8)
C(127)	135(10)	118(8)	105(8)	-22(7)	50(7)	-9(8)
C(128)	167(12)	88(7)	141(10)	-9(7)	39(9)	27(8)
C(129)	248(18)	129(11)	185(14)	-3(10)	95(13)	61(12)
C(130)	240(18)	161(14)	188(15)	-78(12)	90(15)	11(13)
C(131)	275(18)	161(13)	98(9)	-24(9)	72(11)	-59(13)
C(132)	248(17)	136(10)	119(10)	-5(8)	65(11)	-59(12)
C(133)	106(8)	69(5)	66(5)	8(4)	16(5)	-8(5)
C(134)	100(8)	111(7)	86(6)	16(6)	16(6)	-13(6)
C(135)	116(9)	102(7)	77(6)	35(5)	35(6)	24(7)
C(136)	148(11)	91(6)	84(6)	26(5)	68(7)	19(7)
C(137)	138(11)	119(9)	206(14)	76(10)	99(11)	48(8)
C(138)	112(10)	136(10)	148(11)	65(9)	55(8)	34(9)
C(139)	144(11)	108(8)	118(9)	8(7)	58(8)	17(8)
N(140)	96(7)	132(7)	119(6)	56(6)	56(5)	24(6)
C(141)	159(13)	189(15)	221(16)	105(13)	120(12)	46(12)

C(142)	113(15)	135(17)	240(23)	102(16)	101(15)	0(12)
C(143)	186(22)	94(13)	223(23)	35(16)	29(19)	-24(14)
C(144)	234(28)	189(22)	187(22)	48(20)	27(21)	-25(22)
C(145)	294(30)	155(19)	141(19)	30(16)	-17(21)	-99(20)
C(146)	237(24)	122(15)	184(21)	31(15)	61(19)	-57(16)
C(147)	212(21)	182(20)	168(18)	28(16)	118(17)	11(18)
C(150)	196(38)	312(55)	135(27)	-40(31)	-7(25)	147(39)
C(151)	442(90)	447(86)	208(47)	204(55)	175(54)	160(74)
C(152)	181(41)	434(85)	155(32)	23(44)	81(29)	-30(48)
C(153)	219(45)	269(49)	162(32)	-91(34)	23(30)	5(37)
C(154)	335(65)	374(70)	383(73)	-221(60)	-134(55)	243(58)
C(155)	153(16)	296(28)	128(13)	-29(16)	-4(12)	111(17)
C(156)	202(37)	186(36)	168(33)	13(29)	28(27)	-29(29)
C(157)	292(58)	381(71)	119(28)	-79(38)	30(36)	-50(49)
C(158)	181(34)	84(17)	226(39)	49(21)	19(28)	22(20)
C(159)	210(42)	128(22)	124(29)	13(22)	-40(31)	49(26)
C(160)	251(52)	336(61)	254(51)	180(49)	87(45)	36(49)
C(161)	259(60)	458(89)	367(80)	22(68)	61(59)	115(59)
C(162)	284(52)	187(35)	271(47)	-116(34)	85(43)	-34(36)
C(163)	180(32)	327(51)	86(17)	-1(25)	-13(20)	-28(34)
C(164)	356(37)	84(11)	110(14)	-3(9)	23(19)	46(15)
C(169)	226(48)	402(72)	104(26)	-1(35)	54(29)	-6(50)
C(170)	309(48)	113(23)	259(44)	-47(27)	184(40)	-18(29)
C(171)	322(63)	164(31)	117(26)	-43(23)	21(36)	102(34)
C(175)	156(24)	276(39)	268(40)	-115(36)	35(24)	4(27)
C(176)	253(42)	31(9)	171(27)	-31(13)	-8(25)	30(16)
C(177)	256(24)	238(22)	199(18)	0(17)	122(18)	43(20)
C(178)	198(44)	279(60)	315(62)	3(51)	31(45)	-22(43)
C(179)	320(64)	334(60)	224(47)	-188(50)	99(44)	-134(55)
C(180)	115(27)	380(68)	284(50)	-116(47)	-98(30)	-69(36)
C(181)	102(23)	388(62)	227(38)	-51(38)	101(26)	-95(32)
C(182)	324(61)	225(42)	269(48)	149(38)	177(46)	61(39)
C(183)	362(66)	125(29)	201(39)	-82(29)	58(40)	89(38)
C(184)	765(128)	252(50)	119(27)	-18(29)	52(49)	286(70)
C(185)	266(43)	147(24)	147(25)	67(21)	11(27)	-28(27)
C(186)	380(64)	255(50)	332(58)	44(43)	257(53)	164(47)

Table 5. Hydrogen coordinates (x 10^4), isotropic displacement parameters (Å^2 x 10^3) and site occupancy factors for [**1**·**2**]$^{3+}$.

	x	y	z	U(eq)	sof
H(2A)	591(2)	7551(5)	2063(7)	149	1
H(2B)	491(2)	7039(5)	1637(7)	149	1
H(3A)	347(2)	7524(5)	555(8)	181	1
H(3B)	217(2)	7655(5)	1157(8)	181	1
H(5A)	427(7)	8510(6)	1930(22)	215	0.50
H(5B)	171(7)	8404(6)	1364(22)	215	0.50
H(5AA)	154(4)	8434(7)	1177(27)	242	0.50
H(5AB)	187(4)	8556(7)	406(27)	242	0.50
H(6A)	248(3)	9033(6)	613(17)	337	0.50
H(6B)	230(3)	9229(6)	1379(17)	337	0.50
H(6C)	289(3)	9054(6)	1588(17)	337	0.50
H(6D)	220(3)	9249(6)	805(17)	337	0.50
H(8A)	542(3)	9850(6)	683(16)	359	1
H(8B)	423(3)	9952(6)	1318(16)	359	1
H(9A)	759(4)	10387(7)	1547(14)	292	1
H(9B)	791(4)	9953(7)	2142(14)	292	1
H(12A)	1108(4)	10438(6)	2637(10)	384	1
H(13A)	1491(4)	10774(6)	3048(12)	389	1
H(14A)	1794(3)	10672(5)	2526(10)	252	1
H(15A)	1706(3)	10151(5)	1468(9)	249	1
H(18A)	1482(4)	10058(7)	312(10)	307	1
H(18B)	1590(4)	9525(7)	651(10)	307	1
H(19A)	1157(5)	9606(6)	-446(9)	322	1
H(19B)	1406(5)	9534(6)	-620(9)	322	1
H(21A)	1590(4)	8732(6)	-340(14)	243	1
H(21B)	1364(4)	8703(6)	-1033(14)	243	1
H(22A)	1589(5)	8007(6)	-239(14)	344	1
H(22B)	1367(5)	7977(6)	-950(14)	344	1
H(24A)	1131(4)	7224(5)	-439(8)	242	1
H(24B)	1412(4)	7230(5)	-332(8)	242	1
H(25A)	1482(2)	7230(5)	913(6)	167	1
H(25B)	1338(2)	6737(5)	540(6)	167	1
H(28A)	1489(2)	6726(4)	1788(5)	107	1
H(31A)	1781(2)	6408(4)	2459(5)	97	1
H(34A)	2195(2)	6518(4)	2469(6)	130	1
H(34B)	2066(2)	6005(4)	2114(6)	130	1
H(35A)	2444(2)	5592(6)	2465(7)	168	1
H(35B)	2432(2)	6037(6)	1891(7)	168	1
H(37A)	2596(3)	6786(5)	2245(6)	204	1
H(37B)	2814(3)	6423(5)	2233(6)	204	1
H(38A)	2939(2)	7207(5)	2877(9)	201	1
H(38B)	2816(2)	7019(5)	3472(9)	201	1
H(40A)	3228(2)	7080(5)	4297(6)	166	1
H(40B)	3320(2)	7211(5)	3613(6)	166	1
H(41A)	3525(2)	6406(5)	3832(7)	168	1
H(41B)	3636(2)	6854(5)	4389(7)	168	1
H(44A)	3884(3)	6159(8)	4543(11)	228	1
H(45A)	4209(4)	5755(9)	5336(13)	262	1
H(46A)	4196(3)	5428(9)	6448(14)	269	1
H(47A)	3832(3)	5488(7)	6727(8)	197	1
H(50A)	3577(2)	5929(5)	7078(6)	139	1
H(50B)	3458(2)	5404(5)	6742(6)	139	1
H(51A)	3233(2)	5879(5)	7357(5)	133	1
H(51B)	3187(2)	6284(5)	6712(5)	133	1
H(53A)	2759(2)	5888(5)	6694(5)	146	1

H(53B)	2909(2)	5460(5)	7225(5)	146	1
H(54A)	2762(2)	4852(5)	6345(6)	181	1
H(54B)	2550(2)	5133(5)	6553(6)	181	1
H(56A)	2386(2)	4662(4)	5520(6)	131	1
H(56B)	2449(2)	4805(4)	4790(6)	131	1
H(57A)	2037(2)	4933(4)	4716(5)	118	1
H(57B)	2121(2)	5379(4)	5300(5)	118	1
H(60A)	1755(2)	5556(3)	4547(4)	95	1
H(63A)	1419(2)	5437(3)	4691(4)	86	1
H(66A)	1378(2)	5149(4)	5681(6)	133	1
H(66B)	1260(2)	4721(4)	5097(6)	133	1
H(67A)	1004(3)	4498(4)	5809(6)	162	1
H(67B)	1280(3)	4407(4)	6236(6)	162	1
H(69A)	1372(4)	4664(5)	7323(6)	251	1
H(69B)	1104(4)	4581(5)	7328(6)	251	1
H(70A)	1099(3)	5256(5)	7949(7)	238	1
H(70B)	1366(3)	5052(5)	8291(7)	238	1
H(72A)	1593(5)	5818(6)	8589(10)	176	0.50
H(72B)	1328(5)	5904(6)	8636(10)	176	0.50
H(73A)	1524(4)	6517(7)	7760(15)	208	0.50
H(73B)	1545(4)	6659(7)	8587(15)	208	0.50
H(72C)	1133(6)	5668(6)	8797(12)	242	0.50
H(72D)	917(6)	5998(6)	8321(12)	242	0.50
H(73C)	1225(7)	6468(9)	8903(12)	237	0.50
H(73D)	1395(7)	6174(9)	8532(12)	237	0.50
H(76A)	1586(2)	7213(5)	8103(7)	334	1
H(77A)	1602(3)	8068(5)	7765(7)	282	1
H(78A)	1251(3)	8501(6)	7240(7)	322	1
H(79A)	875(3)	8124(4)	7013(7)	319	1
H(82A)	575(4)	7634(9)	6804(15)	399	0.50
H(82B)	590(4)	7602(9)	7643(15)	399	0.50
H(82C)	600(4)	7675(9)	7543(15)	399	0.50
H(82D)	482(4)	7155(9)	7284(15)	399	0.50
H(83A)	405(4)	6832(15)	7467(16)	349	0.50
H(83B)	244(4)	7258(15)	6973(16)	349	0.50
H(83C)	621(6)	7729(11)	6391(17)	271	0.50
H(83D)	360(6)	7755(11)	6411(17)	271	0.50
H(85A)	59(4)	7045(9)	5851(13)	345	0.50
H(85B)	296(4)	7241(9)	5697(13)	345	0.50
H(85C)	86(4)	7172(9)	5749(13)	345	1
H(85D)	220(4)	6713(9)	6184(13)	345	1
H(86A)	16(4)	6436(10)	5096(12)	360	1
H(86B)	125(4)	6866(10)	4714(12)	360	1
H(88A)	132(2)	6178(6)	4025(6)	194	1
H(88B)	275(2)	5689(6)	4417(6)	194	1
H(89A)	437(2)	6091(5)	3516(7)	169	1
H(89B)	524(2)	6542(5)	4092(7)	169	1
H(92A)	782(2)	6402(4)	3376(5)	110	1
H(95A)	808(2)	6843(3)	2590(4)	97	1
H(98A)	1811(2)	7699(3)	3694(5)	99	1
H(10A)	1761(2)	6816(3)	5328(4)	89	1
H(10B)	1174(2)	7499(3)	4025(5)	98	1
H(10C)	1076(2)	8152(4)	3354(5)	127	1
H(10D)	878(2)	8573(4)	2229(6)	124	1
H(10E)	1441(2)	8240(4)	1512(6)	128	1
H(10F)	1620(2)	7796(4)	2581(5)	110	1
H(10G)	902(3)	8939(4)	1100(6)	159	1
H(10H)	1128(3)	8810(4)	821(6)	159	1
H(11B)	764(2)	8141(3)	776(4)	116	1
H(11C)	973(2)	8017(3)	527(4)	116	1
H(11D)	851(3)	8539(6)	-442(7)	209	1
H(11E)	635(3)	8721(6)	-159(7)	209	1

H(11F)	285(4)	8479(7)	-935(14)	285	1
H(11G)	36(2)	7893(11)	-1707(13)	310	1
H(11H)	183(5)	7094(9)	-1873(14)	442	1
H(11I)	579(6)	6882(7)	-1267(18)	560	1
H(11J)	828(3)	7468(10)	-494(14)	514	1
H(11A)	2090(2)	7188(3)	3661(5)	103	1
H(12B)	2474(2)	6924(3)	3849(5)	107	1
H(12C)	2539(2)	6642(4)	5937(5)	111	1
H(12D)	2160(2)	6921(3)	5765(4)	104	1
H(12E)	2874(2)	6494(4)	5507(6)	128	1
H(12F)	2869(2)	6706(4)	4722(6)	128	1
H(12G)	2686(2)	5757(3)	4982(5)	126	1
H(12H)	2629(2)	5962(3)	4233(5)	126	1
H(12I)	3093(2)	5787(4)	5039(6)	142	1
H(12J)	3000(2)	5888(4)	4184(6)	142	1
H(12K)	3076(2)	4963(4)	5518(4)	160	1
H(12L)	3029(3)	4091(4)	5324(6)	217	1
H(13G)	2859(3)	3778(3)	4151(8)	229	1
H(13H)	2735(3)	4337(5)	3171(5)	209	1
H(13I)	2782(3)	5209(5)	3366(4)	198	1
H(13B)	1536(2)	6419(4)	5782(5)	122	1
H(13C)	1307(2)	6077(4)	6448(5)	116	1
H(13D)	785(3)	7035(5)	5496(8)	173	1
H(13E)	949(2)	6203(5)	6916(7)	143	1
H(13F)	721(2)	6474(5)	6374(7)	143	1
H(14B)	898(2)	5529(4)	6136(5)	133	1
H(14C)	705(2)	5786(4)	5573(5)	133	1
H(14D)	641(3)	5512(6)	6899(9)	211	1
H(14E)	435(3)	5692(6)	6201(9)	211	1
H(14F)	534(5)	5067(7)	5112(9)	209	0.661(13)
H(14G)	474(6)	4211(8)	4806(9)	252	0.661(13)
H(14H)	435(5)	3625(5)	5674(14)	257	0.661(13)
H(14I)	457(5)	3895(7)	6847(12)	218	0.661(13)
H(14J)	517(5)	4751(8)	7152(9)	209	0.661(13)
H(14K)	196(9)	5343(14)	5398(28)	160	0.339(13)
H(14L)	21(7)	4631(23)	4730(21)	223	0.339(13)
H(14M)	211(12)	3845(16)	4970(33)	283	0.339(13)
H(14N)	576(11)	3771(15)	5879(38)	415	0.339(13)
H(14O)	750(6)	4482(25)	6547(27)	209	0.339(13)