JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(21), 5140-5141, DOI:10.1021/ja960307r

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Supplementary Table 4. Fractional coordinates and isotropic thermal parameters (Å^2) for the hydrogen atoms of $(C_{42}H_{52}N_4)(C_{16}H_{36}N)^{1+}$ F^-.

Atom	x	y	z	U
H2A	0.3051	-0.0286	-0.0102	0.03023
H3A	0.4485	0.0476	-0.0106	0.02887
H6A	0.5528	0.1610	0.0155	0.03709
H6B	0.5610	0.0949	0.0725	0.03709
H7A	0.6251	0.2612	0.0783	0.0509
H7B	0.6809	0.1798	0.0752	0.0509
H8A	0.6741	0.2329	0.1852	0.063030
H8B	0.6376	0.1411	0.1820	0.063030
H9A	0.5370	0.2890	0.1842	0.04892
H9B	0.5442	0.2258	0.2434	0.04892
H10A	0.4763	0.1214	0.1813	0.03376
H10B	0.4178	0.2006	0.1854	0.03376
H1AA	0.2400	0.1660	0.4483	0.03469
H1AB	0.3321	0.2003	0.4398	0.03469
H2AA	0.2595	0.0894	0.3456	0.09245
H2AB	0.3072	0.0526	0.4050	0.09245
H2AC	0.2639	0.0570	0.3766	0.09245
H2AD	0.3294	0.1144	0.4156	0.09245
H3AA	0.4275	0.1005	0.3356	0.13314
H3AB	0.3603	0.0736	0.2830	0.13314
H4AA	0.4451	-0.0423	0.3105	0.10814
H4AB	0.4187	-0.0322	0.3854	0.10814
H4AC	0.3509	-0.0593	0.3323	0.10814
H1AC	0.2998	0.3337	0.3012	0.03678
H1AD	0.3349	0.2414	0.2927	0.03678
H1N	0.3000(14)	0.1560(14)	0.1248(10)	0.031(6)

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Supplementary Table 5. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of $(C_{42}H_{52}N_4)(C_{16}H_{36}N)^{1+}$ F^-.

1	2	3	1-2	1-2-3
C1	N1	C4	1.376(2)	110.05(14)
C4	N1		1.381(2)	
C2	C1	N1	1.370(3)	107.3(2)
C3	C2	C1	1.421(3)	107.9(2)
C4	C3	C2	1.375(2)	107.6(2)
C5	C4	N1	1.509(2)	121.80(15)
C5	C4	C3		131.1(2)
N1	C4	C3		107.1(2)
C6	C5	C10	1.549(3)	107.87(15)
C6	C5	C4		108.74(15)
C10	C5	C4	1.549(3)	109.05(14)
C7	C6	C5	1.527(3)	114.0(2)
C8	C7	C6	1.525(4)	111.1(2)
C9	C8	C7	1.522(3)	110.7(2)
C10	C9	C8	1.519(3)	111.1(2)
C5	C10	C9		112.8(2)
C1*	C5	C4	1.515(2)	110.5(2)
C1*	C5	C6		110.0(2)
C1*	C5	C10		110.7(2)
C1A	N1A	C1A'	1.524(4)	112.1(2)
C1A'	N1A		1.521(4)	
C2A	C1A	N1A	1.627(5)	109.7(3)
C3A	C2A	C1A	1.477(5)	140.8(3)
C4A	C3A	C2A	1.499(5)	113.3(3)
C1A	N1A	C1A**		105.4(3)
C1A	N1A	C1A'**		110.8(3)
C1A'	N1A	C1A**		110.7(3)
C1A'	N1A	C1A'**		115.9(3)
C1*	C5	C4	1.515(2)	110.5(2)
C1*	C5	C6		110.0(2)
C1*	C5	C10		110.7(2)

Atoms marked by * are related by 0.5-y,x,z. Atoms marked by ** are related by 0.5-x, 0.5-y, z.

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Supplementary Table 6. Bond Lengths (Å) and Angles (°) for the hydrogen atoms of $(C_{42}H_{52}N_4)(C_{16}H_{36}N)^{1+}$ F^-.

1	2	3	1-2	1-2-3
H1N	N1	C1	0.89(2)	125.6(14)
H1N	N1	C4		123.7(14)
H2A	C2	C3	0.96	126.1(2)
H2A	C2	C1		126.0(2)
H3A	C3	C4	0.96	126.1(2)
H3A	C3	C2		126.3(2)
H6A	C6	H6B	0.96	107.8(3)
H6A	C6	C7		109.3(2)
H6A	C6	C5		108.3(2)
H6B	C6	C7	0.96	108.4(2)
H6B	C6	C5		108.9(2)
H7A	C7	H7B	0.96	108.0(3)
H7A	C7	C8		109.2(3)
H7A	C7	C6		108.8(2)
H7B	C7	C8	0.96	109.8(2)
H7B	C7	C6		109.8(3)
H8A	C8	H8B	0.96	108.2(3)
H8A	C8	C9		109.7(3)
H8A	C8	C7		109.6(3)
H8B	C8	C9	0.96	109.2(3)
H8B	C8	C7		109.4(3)
H9A	C9	H9B	0.96	108.1(3)
H9A	C9	C10		109.0(2)
H9A	C9	C8		109.1(2)
H9B	C9	C10	0.96	109.4(2)
H9B	C9	C8		110.0(2)
H10A	C10	H10B	0.96	107.8(2)
H10A	C10	C5		108.9(2)
H10A	C10	C9		108.5(2)
H10B	C10	C5	0.96	108.9(2)
H10B	C10	C9		109.8(2)
H1AA	C1A	H1AB	0.96	108.3(5)
H1AA	C1A	C2A		110.7(4)
H1AA	C1A	H2AD		102.7(4)
H1AA	C1A	N1A		109.7(4)
H1AB	C1A	C2A	0.96	108.8(4)
H1AB	C1A	H2AD		78.9(4)
H1AB	C1A	N1A		109.6(4)
H2AA	C2A	H2AB	0.96	104.9(4)
H2AA	C2A	H2AC		49.7(3)
H2AA	C2A	H2AD		144.2(5)
H2AA	C2A	C3A		102.5(4)
H2AA	C2A	C1A		101.4(3)
H2AB	C2A	H2AC	0.96	55.3(3)
H2AB	C2A	H2AD		66.7(4)

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Supplementary Table 6. (continued).

1	2	3	1-2	1-2-3
H2AB	C2A	C3A		101.0(3)
H2AB	C2A	C1A		102.3(4)
H2AC	C2A	H2AD	0.96	110.6(5)
H2AC	C2A	C3A		112.1(4)
H2AC	C2A	C1A		107.1(4)
H2AD	C2A	C3A	0.96	113.2(4)
H2AD	C2A	C1A		51.2(3)
H3AA	C3A	H3AB	0.96	108.1(6)
H3AA	C3A	C4A		108.7(4)
H3AA	C3A	C2A		108.6(5)
H3AB	C3A	C4A	0.96	109.3(5)
H3AB	C3A	C2A		108.7(4)
H4AA	C4A	H4AB	0.96	109.5(4)
H4AA	C4A	H4AC		109.5(4)
H4AA	C4A	C3A		110.4(4)
H4AB	C4A	H4AC	0.96	109.5(4)
H4AB	C4A	C3A		109.4(4)
H4AC	C4A	C3A	0.96	108.7(4)
H1AC	C1A'	H1AD	0.96	108.9(5)
H1AC	C1A'	N1A		110.7(4)
H1AD	C1A'	N1A	0.96	109.8(4)

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Supplementary Table 7. Torsion Angles (°) for the non-hydrogen atoms of the macrocycle in $(C_{42}H_{52}N_4)(C_{16}H_{36}N)^{1+}$ F^-.

1	2	3	4	1-2-3-4
C1	N1	C4	C3	0.5(3)
C1	N1	C4	C5	-177.0(2)
C4	N1	C1	C2	-0.5(2)
N1	C1	C2	C3	5.(0)
C1	C2	C3	C4	5.(0)
C2	C3	C4	N1	-0.3(4)
C2	C3	C4	C5	176.9(2)
N1	C4	C5	C6	163.3(2)
N1	C4	C5	C10	45.9(2)
C3	C4	C5	C6	-13.5(3)
C3	C4	C5	C10	-130.9(2)
C6	C5	C10	C9	54.3(2)
C10	C5	C6	C7	-53.0(2)
C4	C5	C6	C7	-171.1(2)
C4	C5	C10	C9	172.2(2)
C5	C6	C7	C8	54.8(2)
C6	C7	C8	C9	-55.0(3)
C7	C8	C9	C10	56.9(3)
C8	C9	C10	C5	-58.0(2)
C1*	C5	C4	N1	-75.9(3)
C2*	C1*	C5	C4	-106.3(4)
C2*	C1*	C5	C6	13.7(4)
C2*	C1*	C5	C10	132.8(4)
N1*	C1*	C5	C4	74.7(3)
N1*	C1*	C5	C6	-165.3(4)
N1*	C1*	C5	C10	-46.2(4)

Atoms marked by * are related by 0.5-y, x, z.

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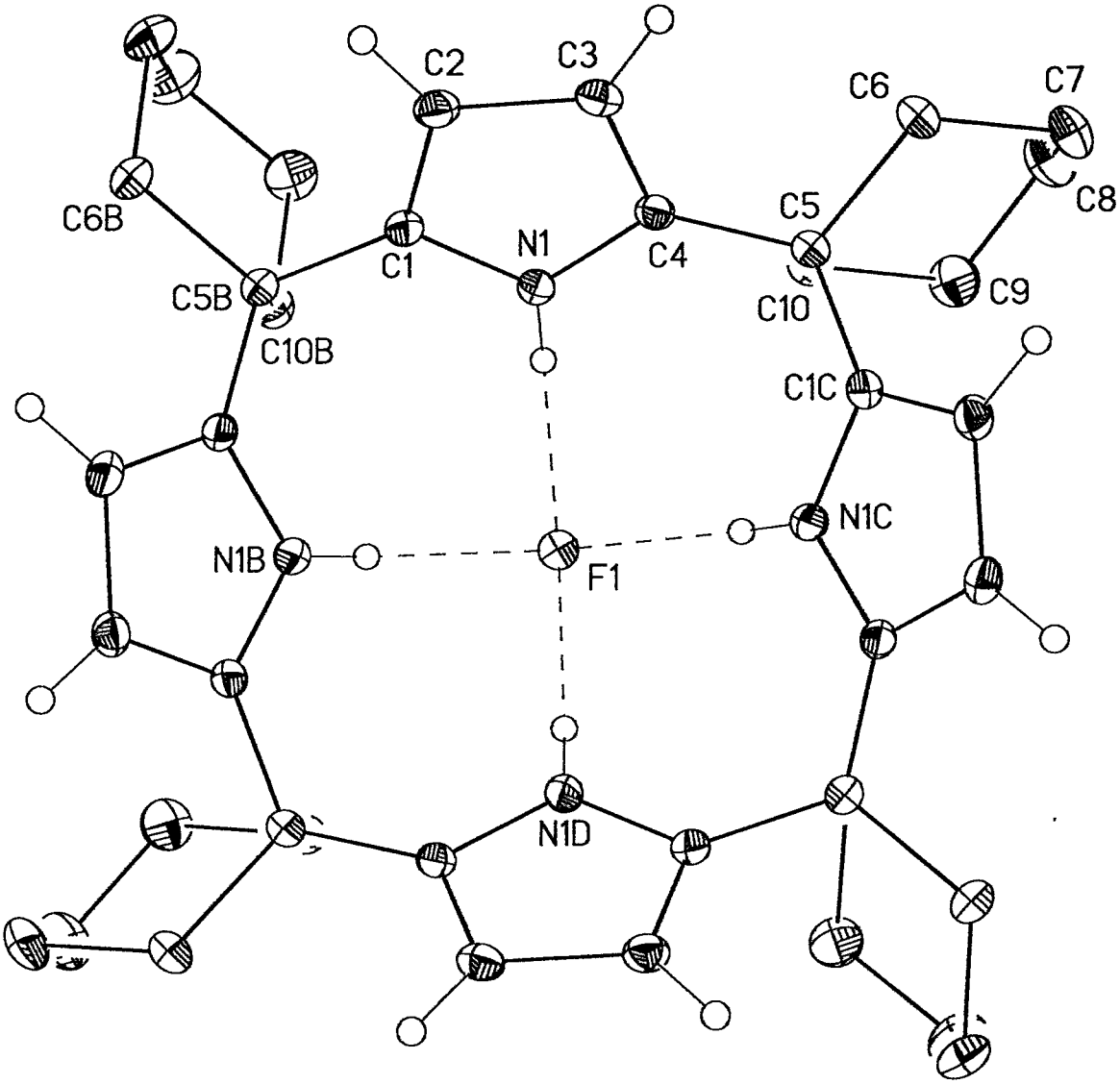

Supplementary Figure 1. View of the ($C_{42}H_{52}N_4$) F^- complex. Thermal ellipsoids are scaled to the 30% probability level. Hydrogen atoms shown are drawn to an arbitrary scale although most have been omitted for clarity. The site symmetry through the macrocycle and the F^- ion is 4mm. The F^- ion is within H-bonding distance of the pyrrolic hydrogen atoms of the porphyrin. The relevant H-bonding distances (Å) and angles (°) are: N1-H1A ··· F1; N ··· F 2.790(2)Å, H ··· F 1.937(2), N-H···F 157.6(3).

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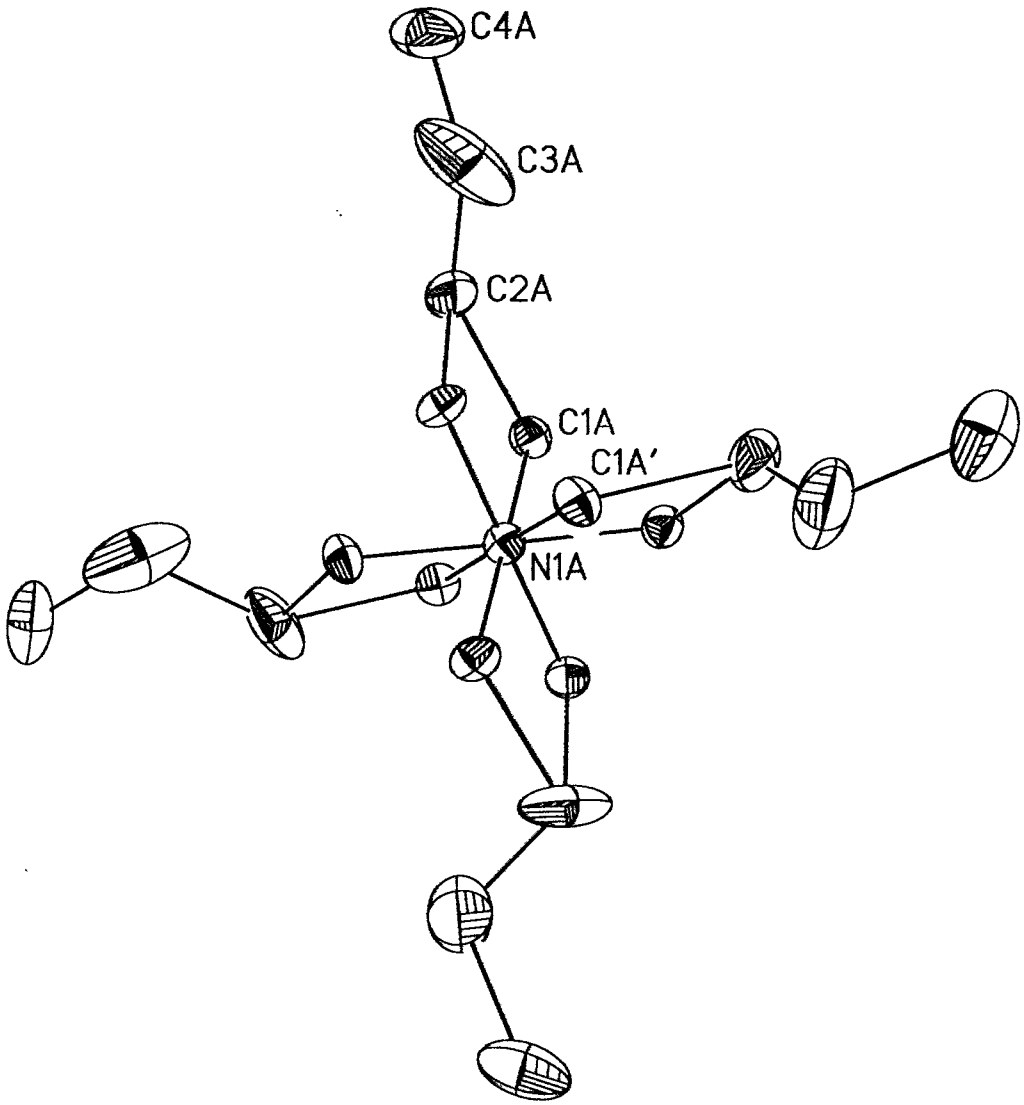
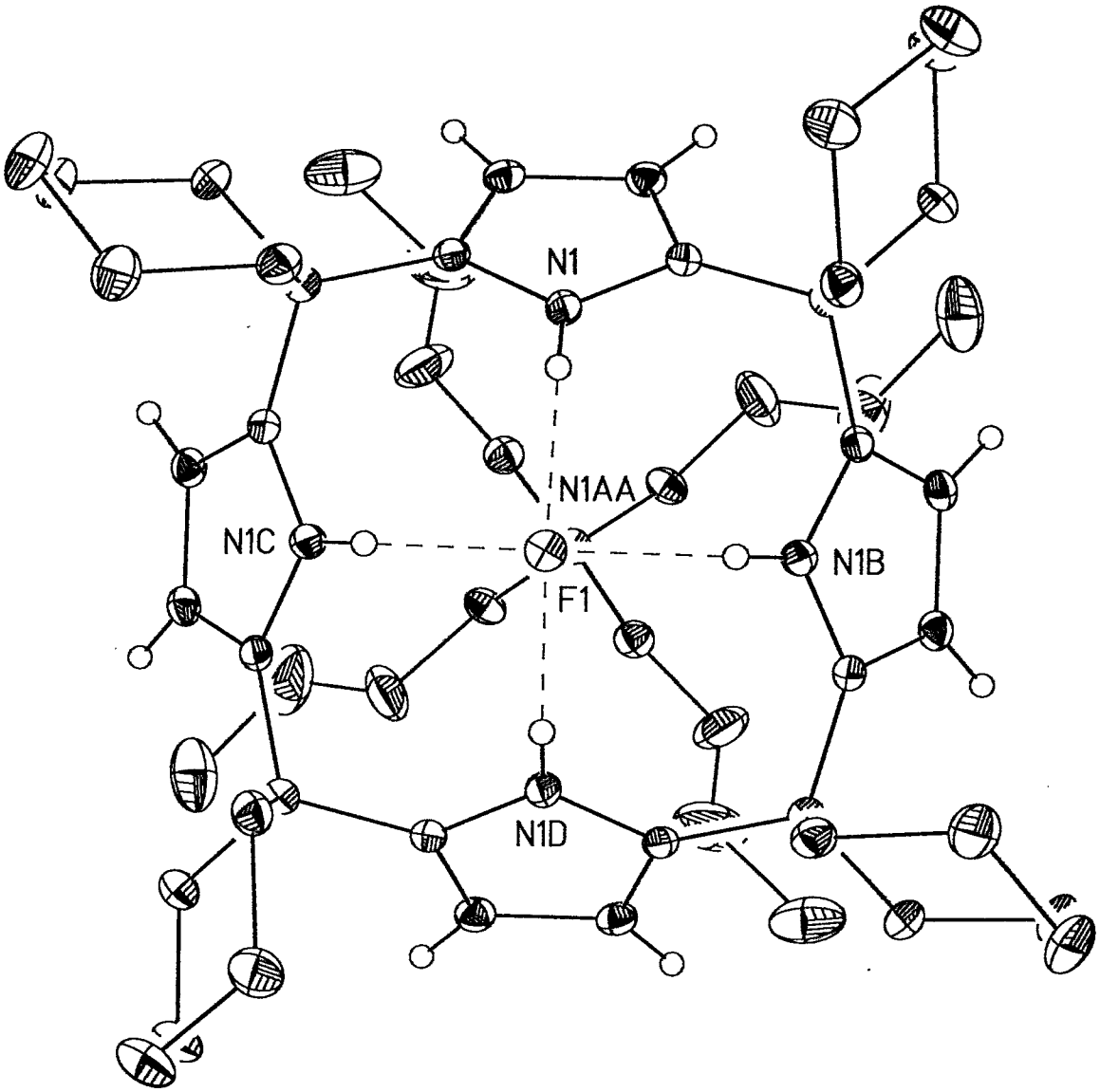


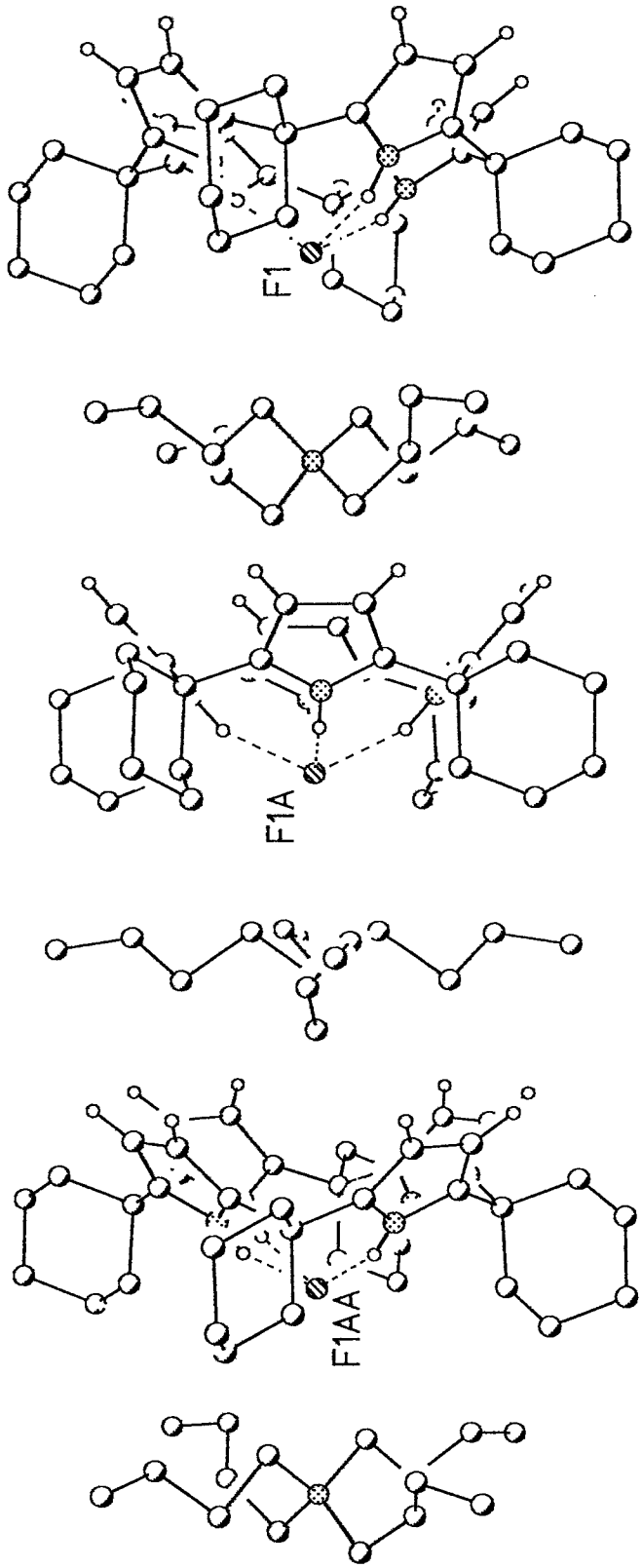
Supplementary Figure 2. View of the tetrakis(n-butyl) ammonium ion. The nitrogen atom, N1A, lies on a crystallographic 4mm symmetry position at 1/4, 1/4, 0.37. The tetrahedral nitrogen cannot have 4mm symmetry and, therefore, must be disordered. The disorder was modeled by allowing for two half-occupancy carbon atoms bound to N1A, C1A and C1A'. The remaining three unique atoms of the cation, C2A, C3A and C4A were refined at full occupancy.

J-5141-88



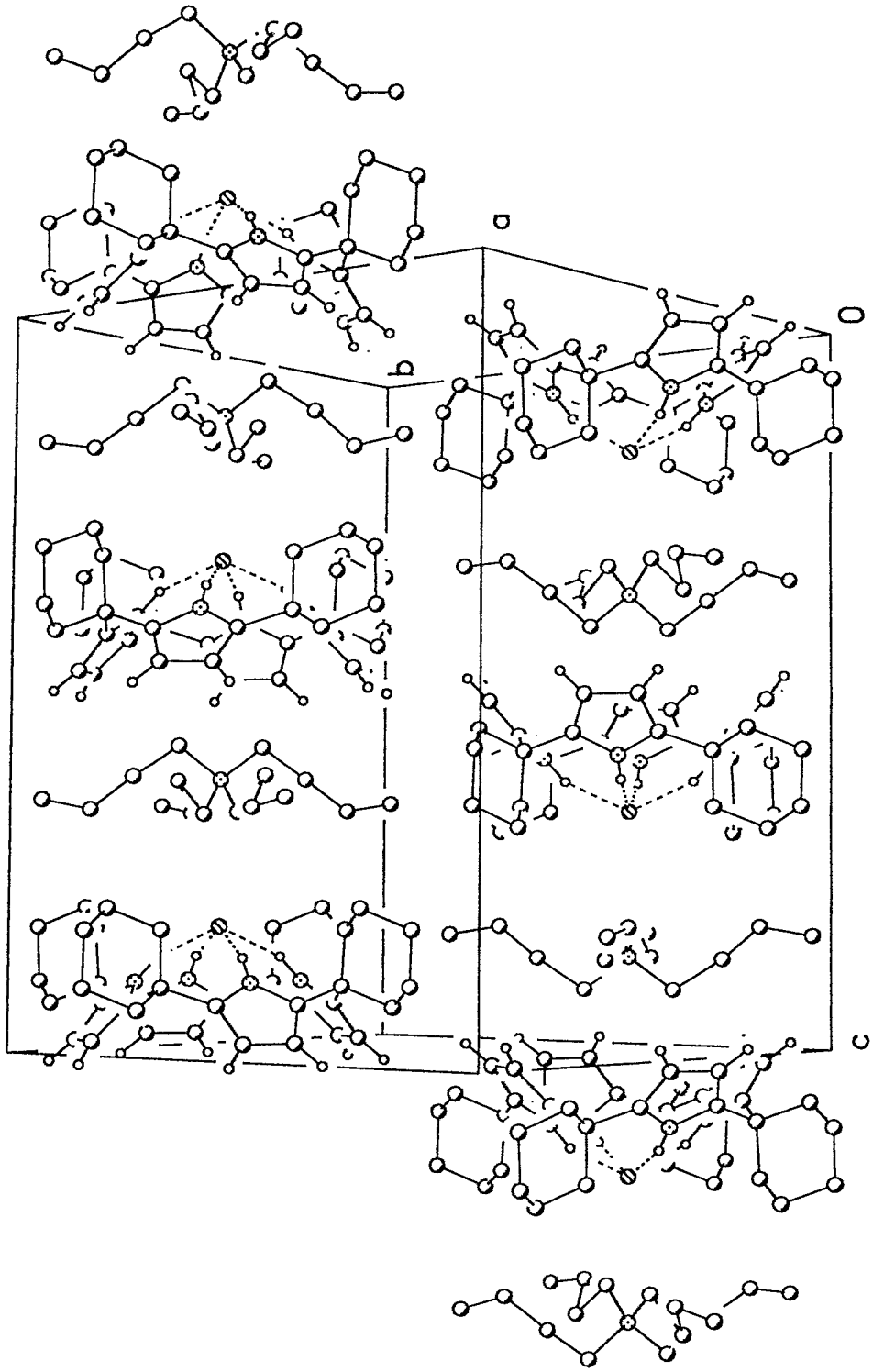
Supplementary Figure 3. View from above the macrocycle showing the interaction of the F^- ion with the pyrrole groups. The cation fits in the grooves between the pyrrole groups. Atom N1AA of the cation is related to N1A in the atom list by 1/2-y, 1/2-x, -1/2+z.

J-5141-89



Supplementary Figure 4. View showing the stacking of the complex. The ammonium ion is closer to the F^- ion from above the macrocycle (4.011(2)Å) than from below it (6.027(2)Å).

J-5141-90



Supplementary Figure 5. Unit cell packing diagram for $(C_{42}H_{52}N_4)(C_{16}H_{36}N)^{1+}$ F^- showing the stacking of the complex along **c**. The view is approximately down the **ab** face diagonal.