Supporting Information

Molecular Recognition of Fluoride Anion: Benzene-based Tripodal Imidazolium Receptor

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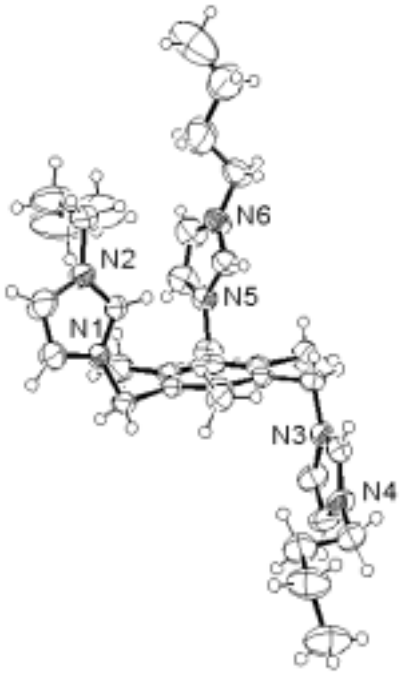

Figure S1. Crystal structure of **2**. The counter ions, PF_6^- ions, have been omitted.

Table S1. Crystal data and structure refinement for compound 2.

Identification code	compound 2	
Empirical formula	C33 H51 F18 N6 P3	
Formula weight	966.71	
Temperature	238(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 19.4354(4) Å	α= 90°.
	b = 9.1274(2) Å	β= 111.51°.
	c = 26.1977(3) Å	γ = 90°.
Volume	4323.54(14) $Å^3$	
Z	4	

Density (calculated)	1.485 Mg/m^3
Absorption coefficient	0.248 mm^{-1}
F(000)	1992
Crystal size	0.15 x 0.25 x 0.50 mm^3
Theta range for data collection	2.25 to 24.14°.
Index ranges	-18<=h<=22, -10<=k<=8, -28<=l<=29
Reflections collected	16835
Independent reflections	6775 [R(int) = 0.1187]
Completeness to theta = 24.14°	98.1 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6775 / 0 / 541
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.1051, wR2 = 0.2656
R indices (all data)	R1 = 0.1494, wR2 = 0.3041
Largest diff. peak and hole	1.007 and -0.574 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	8409(1)	2063(2)	1856(1)	52(1)
P(2)	4545(1)	1530(2)	1127(1)	60(1)
P(3)	1683(1)	4733(2)	1186(1)	60(1)
F(1)	8662(5)	3156(6)	1513(3)	146(3)
F(2)	8111(4)	971(6)	2183(3)	130(2)
F(3)	8829(4)	777(7)	1697(3)	132(2)
F(4)	7922(5)	3267(7)	1964(4)	161(3)
F(5)	7777(4)	1543(10)	1316(3)	157(3)
F(6)	9007(4)	2524(12)	2386(3)	189(4)
F(7)	4379(3)	2651(5)	632(2)	95(2)
F(8)	4844(3)	2851(5)	1540(2)	87(1)
F(9)	4750(3)	397(6)	1616(2)	104(2)
F(10)	5346(3)	1344(8)	1134(3)	128(2)
F(11)	3754(3)	1781(9)	1140(4)	162(3)
F(12)	4235(5)	251(6)	725(2)	177(4)
F(13)	1045(3)	4285(5)	1394(2)	88(2)
F(14)	2150(4)	5260(10)	1796(3)	144(3)
F(15)	2295(4)	5296(8)	973(3)	143(3)
F(16)	1260(4)	4132(12)	619(2)	178(4)
F(17)	1350(5)	6306(7)	1086(4)	158(3)
F(18)	2073(5)	3250(9)	1356(4)	180(4)
N(1)	7922(3)	9235(5)	-56(2)	41(1)
N(2)	8397(3)	11394(6)	27(2)	46(1)
N(3)	6428(3)	7140(6)	1540(2)	42(1)
N(4)	5294(3)	6478(6)	1145(2)	50(1)
N(5)	10147(3)	7210(6)	2131(2)	44(1)
N(6)	10705(3)	9115(6)	2567(2)	56(1)
C(1)	7941(3)	7589(6)	695(2)	39(1)
C(2)	7456(3)	7982(6)	950(2)	37(1)
C(3)	7645(3)	7712(6)	1509(2)	38(1)
C(4)	8320(3)	7071(6)	1816(2)	41(1)
C(5)	8816(3)	6758(6)	1558(2)	42(1)
C(6)	8638(3)	7029(6)	998(2)	40(1)
C(7)	7706(3)	7765(7)	80(2)	45(2)
C(8)	8265(3)	10257(7)	299(2)	44(1)
C(9)	7824(4)	9715(8)	-570(3)	62(2)
C(10)	8127(4)	11068(9)	-513(3)	66(2)
C(11)	8875(4)	12651(7)	291(3)	55(2)
C(12)	9645(5)	12409(11)	317(5)	103(3)
C(13)	10027(7)	11059(15)	602(9)	178(8)
C(14)	10329(14)	10820(20)	1098(5)	249(14)
C(15)	6730(3)	8736(7)	621(2)	49(2)
C(16)	7090(3)	8072(7)	1777(3)	47(2)
C(17)	5734(3)	7609(7)	1353(2)	47(2)
C(18)	6429(4)	5653(8)	1444(3)	56(2)

C(19)	5720(4)	5259(8)	1196(3)	60(2)
C(20)	4490(3)	6586(9)	828(3)	61(2)
C(21)	4333(4)	6850(10)	227(3)	71(2)
C(22)	3511(4)	7053(10)	-114(4)	83(3)
C(23)	3072(5)	5710(10)	-152(4)	95(3)
C(24)	8515(4)	6798(9)	2427(3)	59(2)
C(25)	9569(3)	6088(7)	1884(3)	51(2)
C(26)	10056(3)	8490(8)	2330(3)	51(2)
C(27)	10885(3)	7004(8)	2251(3)	62(2)
C(28)	11230(4)	8189(9)	2521(3)	68(2)
C(29)	10841(4)	10524(9)	2866(3)	69(2)
C(30)	11191(7)	11625(10)	2635(5)	106(3)
C(31)	11392(9)	13055(13)	3025(7)	152(6)
C(32)	11980(8)	13856(14)	2972(5)	140(5)
C(33)	9200(4)	6749(8)	736(3)	58(2)

Table S3. Bond lengths [Å] and angles [°] for compound 2.

P(1)-F(6)	1.508(6)	N(5)-C(26)	1.317(8)
P(1)-F(1)	1.539(5)	N(5)-C(27)	1.365(8)
P(1)-F(4)	1.543(6)	N(5)-C(25)	1.481(8)
P(1)-F(2)	1.559(5)	N(6)-C(26)	1.314(8)
P(1)-F(5)	1.568(6)	N(6)-C(28)	1.366(9)
P(1)-F(3)	1.570(5)	N(6)-C(29)	1.478(9)
P(2)-F(12)	1.540(5)	C(1)-C(2)	1.386(8)
P(2)-F(10)	1.560(6)	C(1)-C(6)	1.393(8)
P(2)-F(11)	1.567(6)	C(1)-C(7)	1.514(8)
P(2)-F(9)	1.579(5)	C(2)-C(3)	1.396(8)
P(2)-F(8)	1.581(5)	C(2)-C(15)	1.522(8)
P(2)-F(7)	1.590(5)	C(3)-C(4)	1.392(8)
P(3)-F(16)	1.511(5)	C(3)-C(16)	1.523(8)
P(3)-F(18)	1.535(7)	C(4)-C(5)	1.395(9)
P(3)-F(17)	1.558(6)	C(4)-C(24)	1.523(8)
P(3)-F(15)	1.573(5)	C(5)-C(6)	1.399(8)
P(3)-F(13)	1.579(5)	C(5)-C(25)	1.526(8)
P(3)-F(14)	1.595(6)	C(6)-C(33)	1.510(9)
N(1)-C(8)	1.313(7)	C(9)-C(10)	1.353(10)
N(1)-C(9)	1.361(8)	C(11)-C(12)	1.489(11)
N(1)-C(7)	1.488(7)	C(12)-C(13)	1.490(17)
N(2)-C(8)	1.337(7)	C(13)-C(14)	1.23(2)
N(2)-C(10)	1.350(8)	C(18)-C(19)	1.340(9)
N(2)-C(11)	1.478(8)	C(20)-C(21)	1.509(11)
N(3)-C(17)	1.326(8)	C(21)-C(22)	1.529(10)
N(3)-C(18)	1.380(8)	C(22)-C(23)	1.476(11)
N(3)-C(16)	1.476(7)	C(27)-C(28)	1.332(10)
N(4)-C(17)	1.324(8)	C(29)-C(30)	1.463(12)
N(4)-C(19)	1.363(9)	C(30)-C(31)	1.615(15)
N(4)-C(20)	1.480(8)	C(31)-C(32)	1.405(17)

F(6)-P(1)-F(1)	93.1(5)	F(10)-P(2)-F(11)	177.2(5)
F(6)-P(1)-F(4)	87.1(6)	F(12)-P(2)-F(9)	88.7(3)
F(1)-P(1)-F(4)	89.7(4)	F(10)-P(2)-F(9)	88.1(3)
F(6)-P(1)-F(2)	89.3(4)	F(11)-P(2)-F(9)	92.1(4)
F(1)-P(1)-F(2)	177.1(5)	F(12)-P(2)-F(8)	178.6(5)
F(4)-P(1)-F(2)	88.7(4)	F(10)-P(2)-F(8)	87.8(4)
F(6)-P(1)-F(5)	177.9(5)	F(11)-P(2)-F(8)	89.5(4)
F(1)-P(1)-F(5)	89.0(4)	F(9)-P(2)-F(8)	91.4(3)
F(4)-P(1)-F(5)	92.9(5)	F(12)-P(2)-F(7)	91.0(3)
F(2)-P(1)-F(5)	88.6(4)	F(10)-P(2)-F(7)	88.9(3)
F(6)-P(1)-F(3)	98.8(6)	F(11)-P(2)-F(7)	91.0(4)
F(1)-P(1)-F(3)	91.3(4)	F(9)-P(2)-F(7)	177.0(3)
F(4)-P(1)-F(3)	174.0(5)	F(8)-P(2)-F(7)	88.9(3)
F(2)-P(1)-F(3)	90.1(3)	F(16)-P(3)-F(18)	89.9(6)
F(5)-P(1)-F(3)	81.2(4)	F(16)-P(3)-F(17)	97.2(6)
F(12)-P(2)-F(10)	93.6(5)	F(18)-P(3)-F(17)	172.9(6)
F(12)-P(2)-F(11)	89.2(5)	F(16)-P(3)-F(15)	88.8(4)

F(18)-P(3)-F(15)	92.0(5)	C(3)-C(2)-C(15)	120.3(5)
F(17)-P(3)-F(15)	87.7(4)	C(4)-C(3)-C(2)	120.6(5)
F(16)-P(3)-F(13)	91.8(3)	C(4)-C(3)-C(16)	120.1(5)
F(18)-P(3)-F(13)	92.2(4)	C(2)-C(3)-C(16)	119.3(5)
F(17)-P(3)-F(13)	88.1(3)	C(3)-C(4)-C(5)	118.6(5)
F(15)-P(3)-F(13)	175.8(4)	C(3)-C(4)-C(24)	119.6(6)
F(16)-P(3)-F(14)	176.2(6)	C(5)-C(4)-C(24)	121.7(5)
F(18)-P(3)-F(14)	86.3(5)	C(4)-C(5)-C(6)	121.5(5)
F(17)-P(3)-F(14)	86.5(5)	C(4)-C(5)-C(25)	120.1(5)
F(15)-P(3)-F(14)	91.7(4)	C(6)-C(5)-C(25)	118.4(6)
F(13)-P(3)-F(14)	87.9(3)	C(1)-C(6)-C(5)	118.5(5)
C(8)-N(1)-C(9)	108.8(5)	C(1)-C(6)-C(33)	121.2(5)
C(8)-N(1)-C(7)	125.9(5)	C(5)-C(6)-C(33)	120.3(6)
C(9)-N(1)-C(7)	125.2(5)	N(1)-C(7)-C(1)	110.4(4)
C(8)-N(2)-C(10)	108.2(5)	N(1)-C(8)-N(2)	108.7(5)
C(8)-N(2)-C(11)	124.3(5)	C(10)-C(9)-N(1)	106.8(6)
C(10)-N(2)-C(11)	126.6(5)	N(2)-C(10)-C(9)	107.6(6)
C(17)-N(3)-C(18)	108.6(5)	N(2)-C(11)-C(12)	110.9(6)
C(17)-N(3)-C(16)	125.5(5)	C(13)-C(12)-C(11)	117.0(10)
C(18)-N(3)-C(16)	125.8(5)	C(14)-C(13)-C(12)	129.2(19)
C(17)-N(4)-C(19)	108.6(5)	N(3)-C(16)-C(3)	109.6(5)
C(17)-N(4)-C(20)	124.7(6)	N(4)-C(17)-N(3)	108.4(6)
C(19)-N(4)-C(20)	125.9(6)	C(19)-C(18)-N(3)	106.5(6)
C(26)-N(5)-C(27)	108.3(5)	C(18)-C(19)-N(4)	107.9(6)
C(26)-N(5)-C(25)	126.6(5)	N(4)-C(20)-C(21)	111.4(6)
C(27)-N(5)-C(25)	124.7(6)	C(20)-C(21)-C(22)	113.4(7)
C(26)-N(6)-C(28)	108.0(6)	C(23)-C(22)-C(21)	113.2(7)
C(26)-N(6)-C(29)	125.7(6)	N(5)-C(25)-C(5)	112.7(5)
C(28)-N(6)-C(29)	126.2(6)	N(6)-C(26)-N(5)	109.1(6)
C(2)-C(1)-C(6)	120.7(5)	C(28)-C(27)-N(5)	107.0(6)
C(2)-C(1)-C(7)	119.5(5)	C(27)-C(28)-N(6)	107.6(6)
C(6)-C(1)-C(7)	119.8(5)	C(30)-C(29)-N(6)	113.6(7)
C(1)-C(2)-C(3)	119.8(5)	C(29)-C(30)-C(31)	109.6(8)
C(1)-C(2)-C(15)	119.9(5)	C(32)-C(31)-C(30)	112.0(10)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	66(1)	48(1)	46(1)	-4(1)	25(1)	-3(1)
P(2)	55(1)	55(1)	47(1)	3(1)	-6(1)	-14(1)
P(3)	59(1)	64(1)	55(1)	-5(1)	19(1)	-12(1)
F(1)	293(9)	76(4)	128(5)	-16(3)	149(6)	-49(5)
F(2)	223(7)	86(4)	126(5)	-19(4)	116(5)	-48(4)
F(3)	182(6)	97(4)	162(6)	22(4)	117(5)	52(4)
F(4)	256(9)	100(5)	198(8)	26(5)	167(8)	72(5)
F(5)	135(6)	187(7)	103(5)	-27(5)	-11(4)	-24(5)
F(6)	149(6)	296(11)	80(4)	-19(6)	-8(4)	-103(7)
F(7)	125(4)	71(3)	55(3)	12(2)	-5(3)	-14(3)
F(8)	113(4)	81(3)	60(3)	-17(2)	23(3)	-16(3)
F(9)	100(4)	106(4)	79(3)	40(3)	-1(3)	-30(3)
F(10)	109(4)	155(6)	148(6)	31(5)	79(4)	43(4)
F(11)	53(3)	190(7)	222(8)	52(6)	28(4)	-12(4)
F(12)	291(10)	68(4)	83(4)	-12(3)	-37(5)	-50(5)
F(13)	100(3)	90(3)	91(3)	-20(3)	56(3)	-37(3)
F(14)	106(4)	209(8)	98(4)	-37(5)	13(4)	-36(5)
F(15)	127(5)	166(6)	183(7)	-42(5)	112(5)	-58(5)
F(16)	128(5)	341(12)	76(4)	-93(6)	51(4)	-126(7)
F(17)	204(7)	92(4)	231(8)	65(5)	145(7)	41(5)
F(18)	206(8)	129(6)	212(9)	40(6)	87(7)	85(6)
N(1)	42(3)	49(3)	26(2)	4(2)	6(2)	-9(2)
N(2)	45(3)	47(3)	44(3)	3(2)	13(2)	-9(2)
N(3)	40(3)	48(3)	34(3)	0(2)	11(2)	-3(2)
N(4)	40(3)	59(3)	50(3)	-2(3)	15(2)	-10(3)
N(5)	36(3)	50(3)	38(3)	2(2)	4(2)	3(2)
N(6)	44(3)	66(4)	50(3)	-14(3)	9(3)	-2(3)
C(1)	46(3)	34(3)	33(3)	-4(2)	11(3)	-11(3)
C(2)	40(3)	34(3)	30(3)	1(2)	5(2)	-10(2)
C(3)	37(3)	39(3)	32(3)	-3(3)	6(2)	-11(2)
C(4)	47(3)	39(3)	31(3)	1(3)	7(3)	-8(3)
C(5)	42(3)	33(3)	39(3)	1(3)	2(3)	-5(2)
C(6)	46(3)	32(3)	40(3)	-3(3)	12(3)	-11(3)
C(7)	53(4)	44(3)	34(3)	-3(3)	12(3)	-16(3)
C(8)	52(4)	48(4)	34(3)	0(3)	16(3)	-9(3)
C(9)	70(5)	75(5)	31(3)	4(3)	6(3)	-23(4)
C(10)	73(5)	72(5)	44(4)	16(4)	9(3)	-20(4)
C(11)	65(4)	44(4)	56(4)	-4(3)	23(3)	-16(3)
C(12)	64(5)	89(7)	153(10)	-36(7)	34(6)	-31(5)
C(13)	71(7)	91(9)	310(20)	-23(13)	-2(10)	-7(6)
C(14)	450(30)	171(16)	64(8)	6(9)	24(13)	-180(20)
C(15)	40(3)	60(4)	36(3)	11(3)	3(3)	-3(3)
C(16)	42(3)	55(4)	40(3)	-7(3)	10(3)	-13(3)
C(17)	50(4)	51(4)	39(3)	-3(3)	17(3)	-3(3)
C(18)	50(4)	50(4)	66(4)	8(3)	18(3)	0(3)

C(19)	60(4)	48(4)	68(5)	-3(3)	19(4)	-21(3)
C(20)	41(4)	75(5)	68(5)	-9(4)	21(3)	-15(3)
C(21)	52(4)	84(6)	70(5)	-9(4)	16(4)	-13(4)
C(22)	68(5)	74(6)	79(6)	-1(5)	-6(4)	-8(4)
C(23)	60(5)	84(6)	119(8)	-15(6)	8(5)	-15(4)
C(24)	51(4)	80(5)	37(4)	12(3)	6(3)	-2(4)
C(25)	51(4)	42(4)	51(4)	3(3)	8(3)	4(3)
C(26)	37(3)	59(4)	50(4)	-7(3)	8(3)	2(3)
C(27)	39(4)	68(5)	72(5)	-7(4)	13(3)	10(3)
C(28)	36(4)	89(6)	68(5)	-12(4)	5(3)	3(4)
C(29)	56(4)	80(5)	63(5)	-24(4)	13(4)	-10(4)
C(30)	143(9)	74(6)	136(9)	-2(6)	92(8)	12(6)
C(31)	222(15)	74(7)	242(17)	-34(9)	181(14)	-19(8)
C(32)	172(13)	113(9)	88(8)	-12(7)	-8(8)	49(9)
C(33)	55(4)	60(4)	62(4)	-12(3)	24(3)	-2(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound 2.

	x	y	z	U(eq)
H(7A)	7940	7004	-65	53
H(7B)	7168	7646	-94	53
H(8A)	8395	10198	682	53
H(9A)	7591	9205	-900	75
H(10A)	8146	11672	-799	79
H(11A)	8877	12783	663	66
H(11B)	8676	13545	82	66
H(12A)	9637	12389	-59	124
H(12B)	9943	13256	501	124
H(13A)	9662	10275	465	214
H(13B)	10409	10865	450	214
H(14A)	10546	9848	1154	374
H(14B)	9965	10881	1270	374
H(14C)	10713	11542	1260	374
H(15A)	6455	8927	858	73
H(15B)	6440	8107	321	73
H(15C)	6831	9654	476	73
H(16A)	7315	7903	2174	56
H(16B)	6949	9107	1717	56
H(17A)	5581	8580	1367	56
H(18A)	6845	5039	1535	67
H(19A)	5546	4309	1078	72
H(20A)	4283	7390	973	73
H(20B)	4249	5676	870	73
H(21A)	4520	6019	80	85
H(21B)	4601	7727	189	85
H(22A)	3314	7835	50	100
H(22B)	3456	7364	-485	100
H(23A)	2557	5904	-371	142
H(23B)	3114	5407	214	142
H(23C)	3255	4937	-322	142
H(24A)	8100	7072	2528	88
H(24B)	8944	7379	2635	88
H(24C)	8626	5767	2506	88
H(25A)	9524	5471	2176	62
H(25B)	9722	5460	1641	62
H(26A)	9600	8892	2306	61
H(27A)	11107	6181	2160	74
H(28A)	11743	8358	2655	82
H(29A)	10369	10912	2862	83
H(29B)	11158	10348	3249	83
H(30A)	10854	11898	2266	127
H(30B)	11642	11220	2606	127
H(31A)	10955	13687	2930	182
H(31B)	11526	12749	3408	182

H(32A)	12093	14688	3220	210
H(32B)	11841	14202	2598	210
H(32C)	12413	13232	3063	210
H(33A)	8988	6997	349	87
H(33B)	9339	5722	776	87
H(33C)	9635	7347	914	87