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Crystal structure of 1,1'-(methane-1,1-diyl)bis(3-propyl-1*H*-imidazol-3-ium) bis(hexafluoridophosphate), $C_{13}H_{22}F_{12}N_4P_2$

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Abstract

$C_{13}H_{22}F_{12}N_4P_2$, monoclinic, $P2_1/c$ (no. 14), $a = 25.252(3)$ Å, $b = 8.3297(9)$ Å, $c = 23.268(2)$ Å, $\beta = 116.271(1)^\circ$, $V = 4388.7(8)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0661$, $wR_{ref}(F^2) = 0.2191$, $T = 296(2)$ K.

CCDC no.: 2100044

One of the two crystallographically independent cations of the title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.21 × 0.13 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.31 mm ⁻¹
Diffractometer, scan mode:	Bruker APEXII, φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	31,566, 7703, 0.042
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 4784
$N(param)_{refined}$:	820
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

Source of material

1-Propylimidazole (4.40 g, 0.04 mol) was dissolved in acetonitrile (25 mL), dibromomethane (3.47 g, 0.02 mol) was quickly added under stirring. The mixture was vigorously stirred at 85 °C for about 12 h. After the reaction completed (monitored by thin layer chromatography (TLC)), a white solid was produced after cooling. The white solid was filtered, crushed, and washed with ethylacetate and diethyl ether three times respectively. Then residual solvent was removed, and the white powder intermediate (C1PM-Br) was dried *in vacuo* (7.6 g, yield 96.57%). Then the intermediates (C1PM-Br) (1.97 g, 0.005 mol), potassium hexafluoro phosphate (2.48 g, 0.012 mol) was dissolved in

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	1.0233 (4)	0.8614 (11)	0.9429 (4)	0.172 (3)
H1A	1.045501	0.832878	0.919980	0.258*
H1B	1.048723	0.913759	0.982282	0.258*
H1C	0.991781	0.932652	0.917208	0.258*
C2	0.9988 (3)	0.7176 (10)	0.9569 (3)	0.142 (3)
H2A	0.962792	0.743509	0.960221	0.170*
H2B	1.026756	0.672069	0.997400	0.170*
C3	0.9859 (3)	0.5989 (8)	0.9038 (2)	0.112 (2)
H3A	1.021212	0.582425	0.897996	0.135*
H3B	0.975015	0.496822	0.915622	0.135*
C4	0.94188 (18)	0.6862 (5)	0.7902 (2)	0.0626 (10)
H4	0.976303	0.680672	0.785052	0.075*
C5	0.8807 (2)	0.6746 (6)	0.8319 (2)	0.0770 (13)
H5	0.865371	0.659753	0.861228	0.092*
C6	0.85070 (19)	0.7198 (6)	0.7710 (2)	0.0739 (12)
H6	0.810482	0.741909	0.749869	0.089*
C7	0.8763 (2)	0.7748 (5)	0.68021 (19)	0.0708 (12)
H7A	0.849239	0.865082	0.667383	0.085*
H7B	0.912365	0.808277	0.678539	0.085*
C8	0.7930 (2)	0.6175 (5)	0.6018 (2)	0.0656 (11)
H8	0.763104	0.681539	0.602427	0.079*
C9	0.8799 (2)	0.5235 (6)	0.6226 (2)	0.0785 (13)
H9	0.920686	0.511897	0.639862	0.094*
C10	0.8394 (2)	0.4272 (6)	0.5795 (2)	0.0820 (13)
H10	0.846830	0.335211	0.561697	0.098*
C11	0.7272 (2)	0.4209 (7)	0.5218 (2)	0.1019 (18)
H11A	0.727840	0.394372	0.481529	0.122*
H11B	0.696775	0.501273	0.513176	0.122*
C12	0.7122 (4)	0.2729 (10)	0.5487 (4)	0.169 (4)
H12A	0.672004	0.242702	0.520017	0.203*
H12B	0.737677	0.186841	0.547722	0.203*
C13	0.7169 (4)	0.2807 (12)	0.6127 (4)	0.200 (4)
H13A	0.756553	0.309470	0.642173	0.300*
H13B	0.707409	0.177857	0.624235	0.300*
H13C	0.689983	0.359941	0.614189	0.300*
N1	0.93778 (15)	0.6541 (4)	0.84307 (16)	0.0663 (9)
N2	0.88943 (14)	0.7277 (4)	0.74541 (14)	0.0544 (8)
N3	0.85003 (15)	0.6419 (4)	0.63617 (15)	0.0575 (8)
N4	0.78511 (16)	0.4880 (5)	0.56651 (15)	0.0681 (9)
C14 ^a	0.8230 (6)	0.0291 (19)	0.8847 (7)	0.156 (5)
H14A ^a	0.815940	−0.044163	0.912347	0.234*
H14B ^a	0.833942	−0.030015	0.856135	0.234*
H14C ^a	0.854409	0.101101	0.910005	0.234*
C15 ^a	0.7690 (6)	0.1219 (19)	0.8471 (8)	0.135 (5)
H15A ^a	0.758140	0.175904	0.877289	0.162*
H15B ^a	0.737793	0.045561	0.823736	0.162*
C14 ^b	0.7618 (7)	0.049 (2)	0.8683 (9)	0.132 (5)
H14D ^b	0.784876	−0.008941	0.907230	0.198*
H14E ^b	0.731089	0.107133	0.872862	0.198*
H14F ^b	0.744407	−0.026094	0.833470	0.198*
C15 ^b	0.8007 (6)	0.163 (2)	0.8549 (9)	0.147 (5)
H15C ^b	0.818697	0.237933	0.890389	0.176*
H15D ^b	0.832038	0.104481	0.850931	0.176*
C16	0.7684 (2)	0.2480 (8)	0.7990 (3)	0.114 (2)
H16A ^a	0.802510	0.317970	0.818184	0.137*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H16B ^a	0.768349	0.197276	0.761411	0.137*
H16C ^b	0.760498	0.179132	0.762439	0.137*
H16D ^b	0.796271	0.328141	0.798981	0.137*
C17	0.7074 (2)	0.4724 (6)	0.8079 (2)	0.0761 (12)
H17	0.738302	0.527764	0.840028	0.091*
C18	0.6584 (2)	0.2953 (6)	0.7371 (2)	0.0786 (13)
H18	0.649047	0.204864	0.711005	0.094*
C19	0.6205 (2)	0.4070 (6)	0.7378 (2)	0.0828 (14)
H19	0.579942	0.408718	0.712066	0.099*
C20	0.6288 (2)	0.6606 (6)	0.7985 (2)	0.0836 (14)
H20A	0.594849	0.698609	0.760711	0.100*
H20B	0.658551	0.744262	0.812386	0.100*
C21	0.5565 (2)	0.6177 (5)	0.8410 (2)	0.0699 (12)
H21	0.523151	0.624970	0.801747	0.084*
C22	0.6470 (2)	0.6110 (6)	0.9134 (2)	0.0824 (14)
H22	0.688053	0.612743	0.933480	0.099*
C23	0.6117 (2)	0.5916 (6)	0.9414 (2)	0.0789 (13)
H23	0.623766	0.577504	0.985085	0.095*
C24	0.5021 (3)	0.5878 (11)	0.9065 (3)	0.147 (3)
H24A ^c	0.471960	0.643352	0.870088	0.176*
H24B ^c	0.490852	0.475423	0.900887	0.176*
H24C ^d	0.503016	0.494716	0.931969	0.176*
H24D ^d	0.467088	0.582012	0.865762	0.176*
C25 ^d	0.5016 (6)	0.7467 (15)	0.9406 (8)	0.118 (4)
H25A ^d	0.536603	0.748307	0.981471	0.141*
H25B ^d	0.505408	0.834161	0.915205	0.141*
C26 ^d	0.4491 (5)	0.7829 (15)	0.9534 (5)	0.124 (4)
H26A ^d	0.454764	0.884628	0.974718	0.186*
H26B ^d	0.413888	0.786586	0.913549	0.186*
H26C ^d	0.445232	0.700320	0.980134	0.186*
C25 ^{rc}	0.4975 (9)	0.8161 (17)	0.9494 (11)	0.109 (4)
H25C ^c	0.492556	0.873449	0.982521	0.164*
H25D ^c	0.535349	0.841429	0.951369	0.164*
H25E ^c	0.466937	0.846860	0.908350	0.164*
C26 ^{rc}	0.4938 (9)	0.6378 (17)	0.9589 (8)	0.136 (4)
H26D ^c	0.524936	0.600550	0.999226	0.163*
H26E ^c	0.455623	0.606052	0.955641	0.163*
N5	0.71300 (16)	0.3392 (5)	0.78178 (17)	0.0711 (10)
N6	0.65214 (16)	0.5170 (4)	0.78272 (16)	0.0646 (9)
N7	0.61133 (16)	0.6278 (4)	0.84918 (15)	0.0615 (8)
N8	0.55593 (16)	0.5959 (4)	0.89612 (17)	0.0695 (9)
F1 ^e	0.6093 (10)	0.706 (3)	0.6353 (10)	0.139 (6)
F2 ^e	0.7246 (7)	0.901 (2)	0.6735 (8)	0.136 (5)
F3 ^e	0.6922 (6)	0.8243 (18)	0.7305 (5)	0.131 (4)
F4 ^e	0.6587 (8)	0.7785 (19)	0.5873 (6)	0.145 (4)
F5 ^e	0.6405 (6)	0.9704 (11)	0.6423 (9)	0.121 (4)
F6 ^e	0.6991 (10)	0.638 (2)	0.6720 (9)	0.129 (5)
F1 ^f	0.6114 (7)	0.739 (2)	0.6580 (7)	0.124 (4)
F2 ^f	0.7238 (5)	0.8658 (15)	0.6497 (6)	0.104 (3)
F3 ^f	0.6642 (6)	0.9012 (18)	0.7032 (6)	0.171 (4)
F4 ^f	0.6597 (7)	0.6967 (15)	0.5914 (7)	0.158 (4)
F5 ^f	0.6257 (4)	0.9306 (14)	0.5993 (5)	0.120 (3)
F6 ^f	0.7047 (6)	0.6669 (17)	0.6961 (6)	0.127 (5)
P1	0.66619 (5)	0.80208 (14)	0.65239 (6)	0.0683 (4)
F7 ^g	0.9228 (2)	0.1680 (6)	0.7031 (2)	0.1183 (15)
F8 ^g	0.9298 (3)	0.2390 (8)	0.8382 (2)	0.1333 (18)

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
F9 ^g	0.88119 (17)	0.3454 (4)	0.7441 (2)	0.1093 (14)
F10 ^g	0.9718 (3)	0.0603 (8)	0.7968 (3)	0.140 (2)
F11 ^g	0.9792 (2)	0.3228 (6)	0.7852 (4)	0.131 (2)
F12 ^g	0.8731 (2)	0.0855 (5)	0.7545 (3)	0.1161 (18)
F7 ^h	0.8755 (11)	0.142 (3)	0.7191 (14)	0.136 (7)
F8 ^h	0.9817 (11)	0.247 (3)	0.8387 (11)	0.149 (6)
F9 ^h	0.8992 (11)	0.316 (3)	0.8052 (16)	0.124 (6)
F10 ^h	0.9640 (12)	0.066 (4)	0.7629 (14)	0.110 (6)
F11 ^h	0.9492 (12)	0.311 (3)	0.7399 (14)	0.123 (6)
F12 ^h	0.9113 (11)	0.071 (3)	0.8121 (13)	0.120 (5)
P2	0.92685 (5)	0.20252 (13)	0.77207 (7)	0.0711 (4)
F13 ⁱ	0.5595 (17)	0.157 (6)	0.7765 (15)	0.124 (7)
F14 ⁱ	0.5868 (17)	0.065 (5)	0.9123 (14)	0.120 (7)
F15 ⁱ	0.6141 (19)	0.242 (5)	0.8845 (18)	0.116 (8)
F16 ⁱ	0.534 (2)	−0.027 (6)	0.806 (2)	0.135 (9)
F17 ⁱ	0.6238 (13)	0.015 (4)	0.845 (2)	0.118 (6)
F18 ⁱ	0.5156 (14)	0.196 (5)	0.8303 (19)	0.126 (7)
F13 ^j	0.5807 (2)	0.0497 (8)	0.7857 (2)	0.1219 (17)
F14 ^j	0.5630 (2)	0.1804 (8)	0.9025 (2)	0.1348 (18)
F15 ^j	0.6276 (2)	0.2289 (7)	0.8642 (2)	0.1068 (16)
F16 ^j	0.5171 (2)	0.0001 (8)	0.8234 (3)	0.128 (2)
F17 ^j	0.6126 (3)	−0.0216 (5)	0.8882 (3)	0.145 (2)
F18 ^j	0.5325 (3)	0.2504 (5)	0.8003 (2)	0.132 (2)
P3	0.57248 (5)	0.11384 (14)	0.84525 (5)	0.0674 (4)
F19 ^k	0.7961 (3)	0.6555 (9)	0.9238 (3)	0.134 (3)
F20 ^k	0.8686 (3)	0.4915 (14)	1.0575 (3)	0.153 (3)
F21 ^k	0.8765 (4)	0.5108 (12)	0.9676 (4)	0.149 (3)
F22 ^k	0.7891 (3)	0.6422 (13)	1.0153 (5)	0.144 (3)
F23 ^k	0.7910 (6)	0.4223 (15)	0.9654 (8)	0.119 (4)
F24 ^k	0.8701 (6)	0.7226 (15)	1.0142 (5)	0.164 (4)
F19A ^l	0.8416 (8)	0.554 (2)	0.9355 (6)	0.132 (4)
F20A ^l	0.8151 (8)	0.557 (2)	1.0520 (6)	0.134 (4)
F21A ^l	0.8651 (6)	0.4034 (14)	1.0163 (9)	0.135 (4)
F22A ^l	0.7889 (6)	0.7081 (16)	0.9717 (10)	0.144 (5)
F23A ^l	0.7746 (9)	0.454 (4)	0.9575 (16)	0.104 (5)
F24A ^l	0.8858 (8)	0.662 (3)	1.0380 (10)	0.138 (6)
P4	0.83213 (5)	0.56915 (16)	0.99287 (5)	0.0728 (4)

^aOccupancy: 0.533(11), ^bOccupancy: 0.467(11), ^cOccupancy:

0.422(10), ^dOccupancy: 0.578(10), ^eOccupancy: 0.447(11),

^fOccupancy: 0.553(11), ^gOccupancy: 0.824(4), ^hOccupancy: 0.176(4),

ⁱOccupancy: 0.135(6), ^jOccupancy: 0.865(6), ^kOccupancy: 0.654(7),

^lOccupancy: 0.346(7).

water (30 mL). The mixture stirred well for 8 h at 105 °C and then cooled slowly. The crystals suitable for X-ray analysis were obtained (yield 78.90%).

Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with C–H = 0.90–0.97 Å with

$U_{iso}(H) = 1.5 U_{eq}(C)$ for methyl H atoms and $1.2 U_{eq}(C)$ for all other H atoms.

Comment

Ionic liquids are composed of organic cations and inorganic or organic anions [5]. Its melting point is 100 °C or lower [6], and it has the advantages of low vapor pressure, non-flammability, good thermal and chemical stability, and great structural adjustability [7, 8]. Carrying out research on ionic liquids is in line with the needs of the development of green chemistry, and is also a topic of common concern for researchers from all over the world in recent years [9, 10]. It is worth mentioning that in recent years, our research group has been devoted to the research of ionic liquids, especially imidazole ionic liquids, and applied them to the catalytic conversion process of biodiesel [11–15]. And reported four crystal structures of 1,1'-(hexane-1,6-diyl)bis(3-ethyl-1*H*-imidazol-3-ium) bis(hexafluoridophosphate), 3-(2-ethoxy-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium hexafluoridophosphate(V), 3,3'-(1,2-phenylenebis(methylene))bis(1-methyl-1*H*-imidazol-3-ium) bis(hexafluoridophosphate), and 3,3'-(1,2-phenylene-bis(methylene)) bis(1-ethyl-1*H*-imidazol-3-ium) bis(hexafluoridophosphate) [16–19]. In order to find an ionic liquid with better catalytic effects and a higher recycling efficiency to catalyze the reaction, we synthesized a new type of imidazole ionic liquid catalyst.

There are two crystallographic independent cations and four crystallographic independent hexafluoridophosphate anions in the asymmetric unit (only one cation is shown in the figure). In the molecule of the title compound bond lengths and angles are very similar to those given in the literature [17–20]. The atoms of imidazole ring are coplanar, and the dihedral angles between the two imidazole rings are 69 and 66°. The torsion angles of C1–C2–C3–N1, C2–C3–N1–C4, C13–C12–C11–N4, C12–C11–N4–C8, C14–C15–C16–N5, C15–C16–N5–C17, C26–C25–C24–N8, and C25–C24–N8–C21 are −67.4(8), 117.2(6), 50.4(9), 70.0(7), −167.9(12), 94.5(8), 175.0(10), and −107.9(8)°, respectively. In the molecule, both propyl groups of 1,1'-(methane-1,1-diyl) bis(3-propyl-1*H*-imidazol-3-ium) cation and four hexafluoridophosphate anions are disordered to some extent. Never the less the structure determination verifies the existence of the title compound.

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