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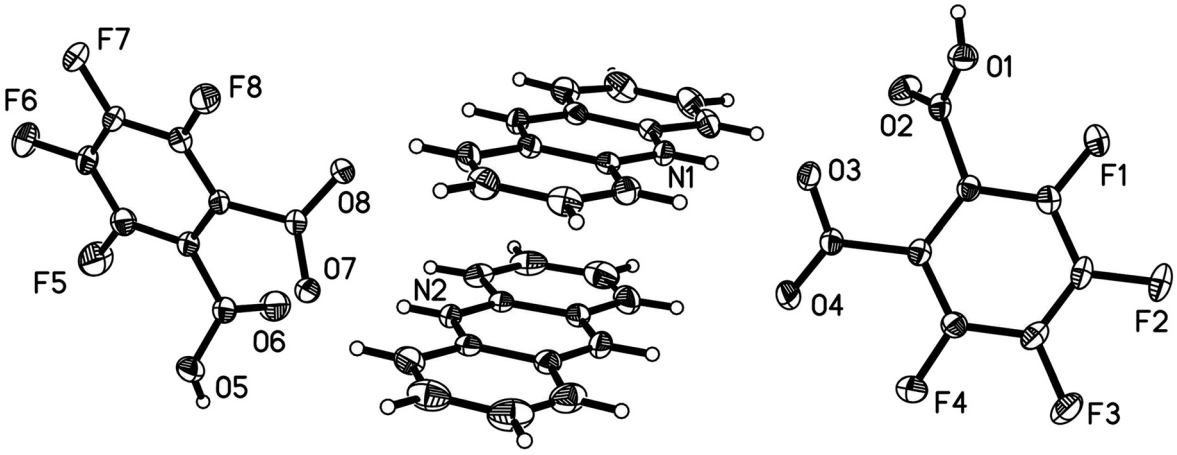
Crystal structure of acrinidinium tetrafluorohydrogenphthalate, $C_{21}H_{11}F_4NO_4$



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Abstract

$C_{21}H_{11}F_4NO_4$, triclinic, $P\bar{1}$ (no. 2), a = 9.5000(4) Å, b = 13.9989(7) Å, c = 14.1423(5) Å, α = 91.355(4)°, β = 108.542(4)°, γ = 98.958(4)°, V = 1756.02(14) Å^3, Z = 4, $R_{gt}(F)$ = 0.0494, $wR_{ref}(F^2)$ = 0.1157, T = 293(2) K.

CCDC no.: 2151627

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:	Orange block
Size:	0.21 × 0.20 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.14 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15,149, 8030, 0.020
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 5734
$N(param)_{refined}$:	543
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3,4]

Source of material

A 3 mL EtOH solution of tetrafluorophthalic acid (TFPA, 23.8 mg, 0.1 mmol) was slowly added into a 3 mL EtOH solution of acridine (AD, 17.9 mg, 0.1 mmol) in a 50 mL beaker. The mixture was stirred for 5 min at room temperature. Orange block crystals of the title compound were obtained after about 10 h (CCDC number 2151627).

Experimental details

Empirical absorption correction was performed using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Using Olex2 [2], the structure was solved with the ShelXT [3] structure solution program and refined with the ShelXL [4] refinement package.

The carbon bound hydrogen atoms were placed in calculated positions and refined using a riding model.

Comment

Over the past few decades, the rational design and synthesis of luminescent materials have attracted great

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
F1	0.69627 (15)	1.12057 (9)	−0.00684 (9)	0.0559 (3)
F2	0.82500 (14)	1.00955 (10)	−0.09927 (8)	0.0531 (3)
F3	0.90785 (15)	0.84375 (10)	−0.02169 (9)	0.0576 (4)
F4	0.87001 (13)	0.79328 (8)	0.14903 (9)	0.0487 (3)
O1	0.71524 (15)	1.16530 (10)	0.19803 (10)	0.0413 (3)
H1B	0.6631	1.2044	0.2057	0.062*
O2	0.50202 (15)	1.05756 (11)	0.16415 (11)	0.0484 (4)
O3	0.72255 (16)	0.96539 (10)	0.31652 (9)	0.0410 (3)
O4	0.70463 (19)	0.81013 (10)	0.27344 (10)	0.0533 (4)
C14	0.74873 (19)	0.92731 (13)	0.16122 (12)	0.0296 (4)
C15	0.70823 (19)	1.01367 (13)	0.12094 (12)	0.0295 (4)
C16	0.7354 (2)	1.03931 (14)	0.03400 (13)	0.0361 (4)
C17	0.8004 (2)	0.98272 (16)	−0.01483 (13)	0.0383 (5)
C18	0.8416 (2)	0.89931 (15)	0.02424 (14)	0.0380 (5)
C19	0.8176 (2)	0.87294 (14)	0.11191 (13)	0.0339 (4)
C20	0.7232 (2)	0.89721 (14)	0.25773 (13)	0.0313 (4)
C21	0.6295 (2)	1.07989 (14)	0.16496 (12)	0.0327 (4)
F5	0.14775 (18)	0.39433 (10)	0.95474 (12)	0.0776 (5)
F6	0.17855 (19)	0.53081 (11)	1.09996 (11)	0.0798 (5)
F7	0.34957 (17)	0.70678 (10)	1.10945 (8)	0.0659 (4)
F8	0.48495 (14)	0.74706 (9)	0.97145 (8)	0.0517 (3)
O5	0.34896 (16)	0.35423 (10)	0.83519 (10)	0.0457 (4)
H5A	0.3167	0.3054	0.7963	0.069*
O6	0.18248 (19)	0.42105 (13)	0.71838 (11)	0.0651 (5)
O7	0.50219 (17)	0.55649 (11)	0.77185 (11)	0.0501 (4)
O8	0.42477 (17)	0.69855 (10)	0.76425 (10)	0.0471 (4)
N1	0.59769 (16)	0.90183 (11)	0.44963 (10)	0.0310 (3)
H1	0.6355	0.9193	0.4037	0.037*
C1	0.8498 (2)	0.90658 (14)	0.55949 (14)	0.0382 (5)
H1A	0.8890	0.9246	0.5088	0.046*
C2	0.9432 (2)	0.89492 (15)	0.65227 (16)	0.0442 (5)
H2	1.0467	0.9046	0.6645	0.053*
C3	0.8857 (2)	0.86837 (16)	0.73020 (15)	0.0469 (5)
H3	0.9518	0.8615	0.7932	0.056*
C4	0.7362 (2)	0.85288 (15)	0.71450 (14)	0.0413 (5)
H4	0.7001	0.8350	0.7665	0.050*
C5	0.2219 (2)	0.84377 (15)	0.47590 (16)	0.0442 (5)
H5	0.1769	0.8273	0.5242	0.053*
C6	0.1349 (2)	0.85265 (17)	0.38120 (18)	0.0524 (6)
H6	0.0305	0.8409	0.3645	0.063*
C7	0.2016 (2)	0.87969 (16)	0.30746 (17)	0.0510 (6)
H7	0.1399	0.8856	0.2428	0.061*
C8	0.3527 (2)	0.89718 (14)	0.32853 (14)	0.0409 (5)
H8	0.3946	0.9159	0.2793	0.049*
C9	0.4779 (2)	0.84906 (14)	0.59706 (13)	0.0358 (4)
H9	0.4373	0.8319	0.6473	0.043*
C10	0.6334 (2)	0.86367 (13)	0.61889 (13)	0.0323 (4)
C11	0.6931 (2)	0.89095 (13)	0.54115 (13)	0.0298 (4)
C12	0.4461 (2)	0.88672 (13)	0.42639 (13)	0.0306 (4)
C13	0.3820 (2)	0.85944 (13)	0.50230 (14)	0.0324 (4)
N2	0.57485 (17)	0.60620 (11)	0.61271 (11)	0.0324 (3)
H2A	0.5481	0.5902	0.6636	0.039*
C22	0.3122 (2)	0.59166 (15)	0.51758 (16)	0.0425 (5)
H22	0.2843	0.5728	0.5726	0.051*
C23	0.2055 (3)	0.59900 (16)	0.42848 (18)	0.0541 (6)
H23	0.1042	0.5849	0.4231	0.065*
C24	0.2453 (3)	0.62744 (17)	0.34429 (18)	0.0597 (7)
H24	0.1702	0.6323	0.2844	0.072*
C25	0.3909 (3)	0.64765 (16)	0.34940 (15)	0.0521 (6)
H25	0.4154	0.6662	0.2931	0.063*
C26	0.9263 (3)	0.66317 (17)	0.5534 (2)	0.0562 (6)
H26	0.9594	0.6793	0.4997	0.067*
C27	1.0271 (3)	0.65335 (19)	0.6427 (2)	0.0654 (7)
H27	1.1291	0.6623	0.6499	0.079*
C28	0.9799 (3)	0.62975 (18)	0.7250 (2)	0.0612 (7)
H28	1.0515	0.6241	0.7863	0.073*
C29	0.8314 (2)	0.61495 (15)	0.71700 (16)	0.0462 (5)
H29	0.8018	0.5995	0.7722	0.055*
C30	0.6602 (2)	0.65850 (14)	0.45079 (15)	0.0430 (5)
H30	0.6893	0.6770	0.3961	0.052*
C31	0.5079 (2)	0.64085 (14)	0.44057 (13)	0.0371 (4)
C32	0.4660 (2)	0.61307 (13)	0.52530 (13)	0.0327 (4)
C33	0.7231 (2)	0.62325 (13)	0.62397 (14)	0.0333 (4)
C34	0.7697 (2)	0.64919 (14)	0.54046 (15)	0.0383 (5)
C35	0.3776 (2)	0.59317 (14)	0.88412 (12)	0.0315 (4)
C36	0.2951 (2)	0.50102 (14)	0.88244 (13)	0.0353 (4)
C37	0.2308 (3)	0.48186 (16)	0.95586 (16)	0.0471 (5)
C38	0.2459 (3)	0.55112 (18)	1.03069 (15)	0.0507 (6)
C39	0.3301 (3)	0.64016 (16)	1.03478 (14)	0.0458 (5)
C40	0.3965 (2)	0.66066 (14)	0.96212 (13)	0.0366 (4)
C41	0.4416 (2)	0.61909 (14)	0.80056 (13)	0.0333 (4)
C42	0.2695 (2)	0.42142 (15)	0.80113 (15)	0.0379 (4)

attention due to their excellent performance in several fields. Among them, two-component crystal materials, assembled by two or more different molecules assembled through hydrogen bond, π–π or charge transfer interactions, have been favored by scientific researchers because of its simple synthetic route, and versatile molecular arrangement [5–9]. It is well known that acrinidine (AD) is an excellent chromophore and fluorinated organic ligand can enhance the luminescence intensity of complex [10–12]. In this work, AD was used as the electron acceptor to react with TFPA, and a complex salt was constructed by forming intermolecular hydrogen bonds.

The asymmetric unit of the title compound consists of two molecules of TFPA anions and two molecules of AD cations. As shown in the figure, one of the carboxyl groups of TFPA is deprotonated and the proton is transfered to the nitrogen atom of AD, and the proton transfer is proved by the comparable C–O bond lengths (C20–O3, 1.253(2) Å; C20–O4, 1.240(2) Å) in the carboxyl group [13,14]. Bond lengths and angles in all ions are in the expected ranges [15,16]. Each AD cation is hydrogen bonded to a TFPA anion by N–H···O hydrogen bond to form a TFPA-AD ion pair,

which is further linked by the O–H···O hydrogen bonds and π–π interactions into a 3D supramolecular structure. From another perspective, the TFPA anions located adjacent to each other are connected through O–H···O hydrogen bonds, forming an infinite 1D chain along the b direction, and the AD cations are fixed together by multiple TFPA chains in an antiparallel packing manner through N–H···O hydrogen bonds and π–π interactions, forming a 3D supramolecular structure.

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