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4,4′-Bipyridine–2,3,4,5,6-pentafluorobenzoic acid (1/2)

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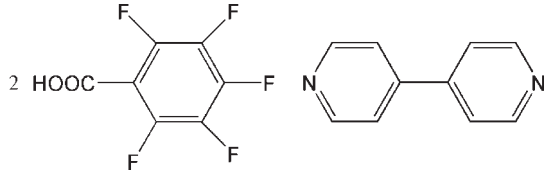
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 14.7.

In the title 1:2 adduct, $C_{10}H_8N_2\cdot 2C_7HF_5O_2$, the complete 4,4′-bipyridine molecule is generated by a crystallographic twofold axis. The components of the adduct are linked by intermolecular O—H···N hydrogen bonds and further connected by a combination of C—H···O, C—H···F and F···F [2.859 (2) Å] interactions.

Related literature

For further discussion of intermolecular interactions involving fluorine atoms, see, for example: Chopra & Row (2008); Choudhury & Row (2004).



Experimental

Crystal data

$C_{10}H_8N_2\cdot 2C_7HF_5O_2$
M_r = 580.34
Monoclinic, $C2/c$
a = 17.910 (3) Å
b = 10.7016 (19) Å
c = 13.498 (3) Å
β = 119.631 (3)°
V = 2248.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 296 K
0.30 × 0.28 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.946, T_{max} = 0.974
6884 measured reflections
2695 independent reflections
2060 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.05
2695 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1	0.82	1.78	2.602 (2)	176
C9—H9···O1	0.93	2.40	3.102 (2)	132
C10—H10···O1^{i}	0.93	2.35	3.196 (2)	152
C12—H12···F5^{ii}	0.93	2.48	3.126 (2)	127
C13—H13···F5^{ii}	0.93	2.63	3.214 (2)	121

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+2, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5082).

References

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