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

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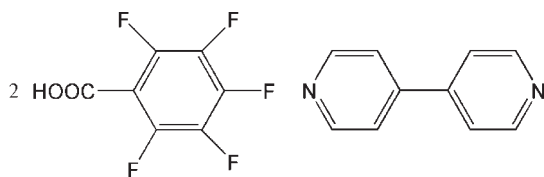
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 14.7.

In the title 1:2 adduct, $\text{C}_{10}\text{H}_8\text{N}_2 \cdot 2\text{C}_7\text{HF}_5\text{O}_2$, the complete 4,4'-bipyridine molecule is generated by a crystallographic twofold axis. The components of the adduct are linked by intermolecular $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds and further connected by a combination of $\text{C}-\text{H} \cdots \text{O}$, $\text{C}-\text{H} \cdots \text{F}$ and $\text{F} \cdots \text{F}$ [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

$\text{C}_{10}\text{H}_8\text{N}_2 \cdot 2\text{C}_7\text{HF}_5\text{O}_2$
 $M_r = 580.34$
 Monoclinic, $C2/c$

$a = 17.910$ (3) Å
 $b = 10.7016$ (19) Å
 $c = 13.498$ (3) Å

$\beta = 119.631$ (3)°
 $V = 2248.8$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.17$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.28 \times 0.20$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

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, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O2}-\text{H2} \cdots \text{N1}$	0.82	1.78	2.602 (2)	176
$\text{C9}-\text{H9} \cdots \text{O1}$	0.93	2.40	3.102 (2)	132
$\text{C10}-\text{H10} \cdots \text{O1}^i$	0.93	2.35	3.196 (2)	152
$\text{C12}-\text{H12} \cdots \text{F5}^{ii}$	0.93	2.48	3.126 (2)	127
$\text{C13}-\text{H13} \cdots \text{F5}^{ii}$	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).

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