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Supplementary Material

Isolation and Structure of a Hydrogen-bonded 2,2′:6′,2′′-Terpyridin-4′-one Acetic Acid Adduct

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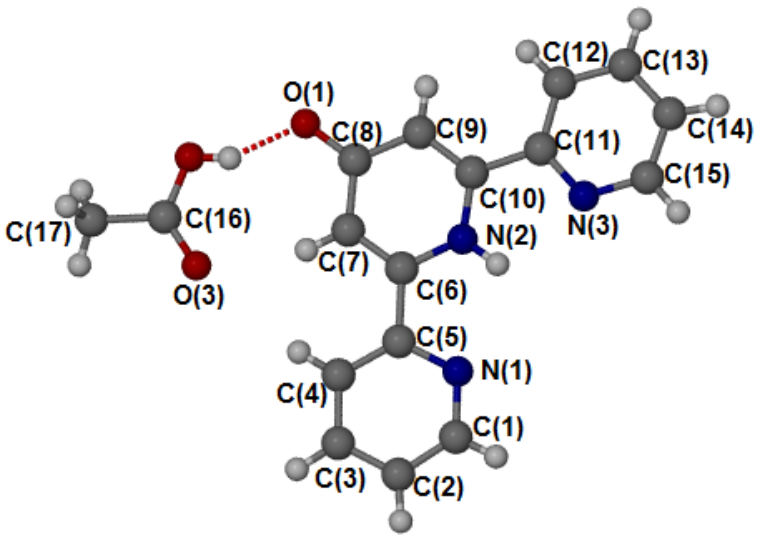

Figure 1: Crystal structure of the hydrogen bonded complex **4** between the terpyridin-4'-one and acetic acid showing atom numbering.

Table 1. Selected interatomic distances (Å) from the X-ray structure of **4**.

Bond	Distance (Å)	Bond	Distance (Å)
N1—C1	1.332 (2)	C6—C5	1.483 (2)
N1—C5	1.345 (2)	C7—C6	1.359 (2)
N2—C10	1.358 (2)	C7—C8	1.419 (3)
N2—C6	1.362 (2)	C9—C8	1.422 (2)
N3—C15	1.338 (2)	C10—C9	1.368 (2)
N3—C11	1.343 (2)	C10—C11	1.481 (2)
O1—C8	1.277 (2)	C11—C12	1.385 (2)
O2—C16	1.306 (2)	C12—C13	1.378 (3)
C2—C1	1.374 (3)	C14—C15	1.366 (3)
C3—C2	1.380 (3)	C14—C13	1.379 (3)
C4—C3	1.378 (3)	C16—O3	1.211 (2)
C5—C4	1.386 (3)	C16—C17	1.499 (3)

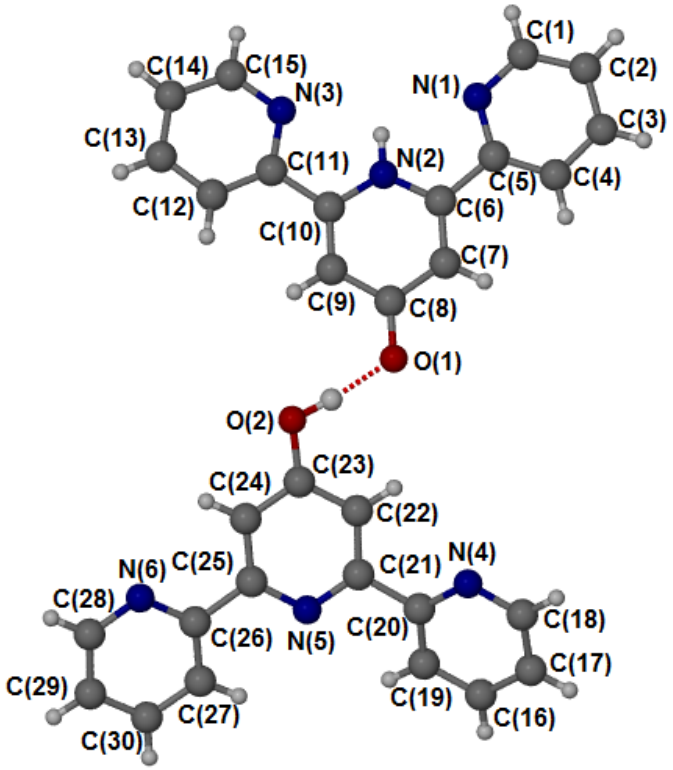

Figure 2: Crystal structure of the hydrogen bonded keto-enol dimer of **2** showing atom numbering.

Table 2. Selected interatomic distances (Å) from the X-ray structure of **2**.

Enol Tautomer		Keto Tautomer	
Bond	Distance (Å)	Bond	Distance (Å)
O1—C8	1.2644 (17)	O2—C23	1.3453 (16)
N1—C1	1.3330 (18)	N5—C21	1.3408 (17)
N1—C5	1.340 (2)	N5—C25	1.3424 (18)
C2—C1	1.377 (2)	C22—C23	1.387 (2)
C2—C3	1.376 (2)	C22—C21	1.3883 (19)
C4—C3	1.386 (2)	C24—C23	1.3924 (18)
C5—C4	1.383 (2)	C24—C25	1.3800 (19)
N2—C6	1.3533 (19)	N4—C16	1.333 (2)
N2—C10	1.3573 (17)	C20—N4	1.3379 (19)
C7—C6	1.358 (2)	C18—C17	1.375 (2)
C7—C8	1.4340 (19)	C19—C18	1.380 (2)
C9—C10	1.364 (2)	C16—C17	1.378 (2)
C9—C8	1.427 (2)	C20—C19	1.384 (2)

Torsion angles -11.2° for C24,C25,C26,N6 and +24.7° for C22,C21,C20,N4 in the enol tautomer.