

A unique co-crystallization motif for bis(4-pyridyl)acetylene involving S \cdots spC interactions with a fused 1,3-dithiole ring

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Table S1: Selected bond lengths (Å) of co-crystal 4.

Bond	Distance (Å)
C(1)–O(1)	1.198(3)
C(1)–S(1)	1.775(2)
C(1)–S(2)	1.789(2)
N(1)–C(8)	1.341(3)
N(1)–C(9)	1.338(3)
N(2)–C(13)	1.336(3)
N(2)–C(14)	1.324(3)
C(16)–C(16#)	1.199(4)
C(16)–C(17)	1.433(3)
N(3)–C(19)	1.326(3)
N(3)–C(20)	1.340(3)

Table S2: Selected bond angles (°) of co-crystal 4.

Bond	Angle(°)
C(1)–S(2)–C(3)	95.74(11)
C(1)–S(1)–C(2)	95.75(10)
C(3)–S(4)–C(5)	100.61(10)
C(2)–S(3)–C(4)	100.03(10)
S(4)–C(5)–C(11)	113.19(14)
S(3)–C(4)–C(6)	112.64(13)
C(14)–N(2)–C(13)	116.28(18)
C(8)–N(1)–C(9)	116.12(19)
C(20)–N(3)–C(19)	116.1(19)