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Supporting information for article:

A temperature-induced order-disorder phase transition in a novel 4-substituted 4,2':6',4''-terpyridine

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Table S1 Bond distances (Å)

Bond	170 K		220 K		274 K		277 K	293 K
	IIA	IIB	IIA	IIB	IIA	IIB	I(A)	I(A)
N1—C3	1.329 (2)	1.330 (2)	1.328 (2)	1.330 (2)	1.323 (3)	1.319 (3)	1.327 (3)	1.324 (3)
N1—C2	1.3399 (19)	1.338 (2)	1.335 (2)	1.330 (2)	1.339 (3)	1.322 (3)	1.331 (3)	1.327 (3)
N2—C6	1.3404 (18)	1.3402 (17)	1.3398 (19)	1.3438 (19)	1.337 (2)	1.341 (2)	1.3385 (17)	1.3360 (17)
N2—C10	1.3421 (17)	1.3439 (17)	1.3419 (19)	1.3406 (19)	1.340 (2)	1.339 (2)	1.3409 (18)	1.3392 (18)
N3—C14	1.3350 (19)	1.3333 (19)	1.332 (2)	1.333 (2)	1.327 (3)	1.325 (3)	1.317 (2)	1.317 (2)
N3—C13	1.334 (2)	1.337 (2)	1.331 (2)	1.332 (2)	1.326 (3)	1.321 (3)	1.323 (2)	1.319 (2)
N4—C18	1.316 (2)	1.314 (2)	1.309 (2)	1.313 (2)	1.313 (3)	1.316 (3)	1.313 (2)	1.309 (2)
N4—C17	1.3679 (19)	1.3651 (19)	1.366 (2)	1.366 (2)	1.367 (3)	1.369 (3)	1.367 (2)	1.363 (2)
C1—C2	1.3822 (19)	1.3776 (19)	1.378 (2)	1.375 (2)	1.379 (3)	1.381 (3)	1.376 (3)	1.373 (3)
C1—C5	1.393 (2)	1.390 (2)	1.393 (2)	1.388 (2)	1.384 (3)	1.382 (3)	1.388 (3)	1.382 (3)
C3—C4	1.3900 (19)	1.388 (2)	1.386 (2)	1.385 (2)	1.387 (3)	1.385 (3)	1.390 (3)	1.388 (3)
C4—C5	1.387 (2)	1.388 (2)	1.387 (2)	1.387 (2)	1.382 (3)	1.375 (3)	1.384 (3)	1.382 (3)
C5—C6	1.4901 (18)	1.4925 (18)	1.489 (2)	1.488 (2)	1.492 (2)	1.491 (2)	1.496 (4)	1.496 (4)
C6—C7	1.3953 (19)	1.3915 (19)	1.391 (2)	1.396 (2)	1.391 (3)	1.389 (3)	1.3917 (19)	1.390 (2)
C7—C8	1.3917 (18)	1.3925 (18)	1.388 (2)	1.385 (2)	1.389 (2)	1.384 (2)	1.3893 (18)	1.3879 (19)
C8—C9	1.390 (2)	1.385 (2)	1.386 (2)	1.385 (2)	1.386 (3)	1.382 (3)	1.3829 (19)	1.381 (2)
C8—C16	1.495 (2)	1.4960 (19)	1.493 (2)	1.496 (2)	1.493 (3)	1.495 (3)	1.4900 (19)	1.4925 (19)
C9—C10	1.393 (2)	1.3911 (19)	1.390 (2)	1.390 (2)	1.388 (3)	1.391 (3)	1.3915 (19)	1.3917 (19)
C10—C11	1.488 (2)	1.487 (2)	1.489 (2)	1.487 (2)	1.487 (3)	1.486 (3)	1.4870 (19)	1.4884 (19)
C11—C12	1.3893 (19)	1.386 (2)	1.386 (2)	1.383 (2)	1.378 (3)	1.379 (3)	1.376 (2)	1.373 (2)
C11—C15	1.388 (2)	1.3900 (19)	1.385 (2)	1.383 (2)	1.378 (3)	1.378 (3)	1.378 (2)	1.376 (2)

C12—C13	1.377 (2)	1.377 (2)	1.375 (2)	1.376 (2)	1.376 (3)	1.378 (3)	1.377 (2)	1.373 (2)
C14—C15	1.375 (2)	1.378 (2)	1.372 (2)	1.375 (2)	1.370 (3)	1.372 (3)	1.374 (2)	1.374 (2)
C16—C17	1.365 (2)	1.367 (2)	1.364 (2)	1.365 (2)	1.353 (3)	1.358 (3)	1.361 (2)	1.361 (2)
C16—C24	1.425 (2)	1.422 (2)	1.421 (2)	1.421 (2)	1.423 (3)	1.420 (3)	1.418 (2)	1.415 (2)
C18—C19	1.416 (2)	1.412 (2)	1.416 (2)	1.409 (2)	1.406 (3)	1.402 (3)	1.406 (2)	1.407 (3)
C19—C20	1.414 (2)	1.416 (2)	1.415 (2)	1.413 (2)	1.413 (3)	1.418 (3)	1.412 (2)	1.411 (2)
C19—C24	1.4146 (19)	1.415 (2)	1.415 (2)	1.415 (2)	1.415 (3)	1.411 (3)	1.415 (2)	1.415 (2)
C20—C21	1.365 (2)	1.360 (2)	1.361 (2)	1.356 (3)	1.350 (4)	1.341 (4)	1.352 (3)	1.347 (3)
C21—C22	1.405 (2)	1.405 (2)	1.408 (3)	1.405 (3)	1.402 (3)	1.403 (4)	1.408 (3)	1.408 (3)
C22—C23	1.363 (2)	1.367 (2)	1.365 (2)	1.360 (3)	1.357 (3)	1.360 (3)	1.358 (2)	1.361 (3)
C23—C24	1.410 (2)	1.414 (2)	1.409 (2)	1.412 (2)	1.405 (3)	1.398 (3)	1.408 (2)	1.409 (2)

Table S2 Bond angles (°)

Angles	170 K		220 K		274 K		277 K	293 K
	IIA	IIB	IIA	IIB	IIA	IIB	I(A)	I(B)
C3—N1—C2	115.99 (13)	115.54 (13)	115.63 (15)	115.29 (15)	115.66 (19)	114.76 (19)	115.75 (19)	115.5 (2)
C10—N2—C6	118.32 (12)	118.65 (12)	118.47 (13)	118.70 (13)	118.50 (17)	118.52 (16)	118.54 (12)	118.59 (12)
C13—N3—C14	115.30 (14)	115.37 (14)	115.13 (15)	115.04 (16)	115.1 (2)	115.0 (2)	114.84 (14)	114.74 (15)
C18—N4—C17	116.85 (13)	116.63 (14)	116.68 (15)	116.52 (16)	116.1 (2)	116.1 (2)	116.34 (15)	116.44 (15)
C5—C1—C2	119.37 (14)	119.43 (14)	119.49 (17)	119.66 (16)	119.8 (2)	119.2 (2)	119.5 (2)	119.7 (2)
N1—C2—C1	123.99 (15)	124.39 (15)	124.30 (18)	124.64 (17)	123.8 (2)	125.1 (2)	124.3 (2)	124.5 (2)
N1—C3—C4	124.45 (14)	124.64 (15)	124.74 (17)	124.71 (17)	124.7 (2)	125.0 (2)	124.6 (2)	124.7 (2)
C5—C4—C3	118.99 (14)	118.96 (14)	119.04 (17)	119.12 (16)	119.1 (2)	119.4 (2)	118.7 (2)	118.8 (2)
C1—C5—C4	117.12 (13)	116.99 (13)	116.73 (15)	116.51 (15)	116.78 (18)	116.40 (18)	117.05 (18)	116.80 (19)
C1—C5—C6	122.93 (13)	123.16 (13)	123.11 (15)	123.40 (15)	123.04 (19)	123.80 (19)	122.6 (4)	122.3 (4)
C4—C5—C6	119.95 (13)	119.85 (13)	120.16 (15)	120.09 (14)	120.17 (19)	119.77 (19)	120.3 (4)	120.8 (4)
N2—C6—C7	122.97 (12)	122.48 (12)	122.47 (14)	122.12 (14)	122.95 (17)	122.34 (16)	122.54 (12)	122.51 (13)
N2—C6—C5	115.06 (12)	114.90 (12)	115.09 (14)	114.96 (13)	114.73 (17)	114.80 (17)	112.1 (2)	112.6 (3)
C7—C6—C5	121.91 (13)	122.62 (13)	122.37 (14)	122.91 (14)	122.29 (18)	122.86 (18)	125.0 (3)	124.5 (3)
C8—C7—C6	118.60 (13)	118.83 (13)	119.24 (15)	119.08 (15)	118.68 (19)	119.28 (18)	119.00 (13)	118.99 (13)
C9—C8—C7	118.44 (13)	118.45 (13)	118.09 (15)	118.54 (15)	118.12 (18)	118.23 (18)	118.17 (13)	118.27 (13)
C9—C8—C16	119.42 (12)	118.90 (12)	119.49 (14)	118.70 (14)	119.68 (17)	119.08 (16)	119.44 (12)	119.40 (12)
C7—C8—C16	122.11 (13)	122.61 (13)	122.40 (15)	122.72 (15)	122.18 (19)	122.68 (18)	122.39 (13)	122.33 (13)
C8—C9—C10	119.41 (12)	119.50 (13)	119.57 (14)	119.43 (14)	119.91 (17)	119.60 (17)	119.73 (13)	119.59 (13)
N2—C10—C9	122.25 (13)	122.08 (13)	122.16 (15)	122.12 (15)	121.84 (18)	122.03 (18)	122.02 (13)	122.04 (13)

N2—C10—C11	116.25 (12)	116.25 (12)	116.16 (14)	116.16 (14)	116.16 (17)	116.01 (17)	116.02 (12)	116.07 (12)
C9—C10—C11	121.50 (12)	121.57 (12)	121.68 (14)	121.64 (14)	122.00 (17)	121.90 (16)	121.95 (12)	121.89 (13)
C12—C11—C15	116.49 (13)	116.42 (13)	116.33 (15)	116.28 (15)	116.10 (19)	115.88 (19)	115.87 (14)	115.80 (14)
C12—C11—C10	121.66 (13)	122.21 (13)	121.73 (15)	122.33 (14)	121.78 (19)	122.47 (18)	122.44 (13)	122.55 (13)
C15—C11—C10	121.84 (12)	121.32 (13)	121.94 (14)	121.35 (15)	122.13 (17)	121.63 (17)	121.68 (13)	121.63 (13)
C11—C12—C13	119.59 (14)	119.79 (14)	119.75 (16)	120.01 (16)	119.7 (2)	120.0 (2)	120.06 (15)	120.15 (16)
N3—C13—C12	124.44 (14)	124.22 (14)	124.44 (16)	124.28 (17)	124.6 (2)	124.4 (2)	124.61 (15)	124.64 (16)
N3—C14—C15	124.70 (15)	124.69 (15)	124.86 (16)	124.92 (17)	124.5 (2)	124.9 (2)	125.09 (16)	125.16 (16)
C14—C15—C11	119.44 (13)	119.48 (14)	119.47 (15)	119.44 (16)	120.02 (19)	119.77 (19)	119.51 (15)	119.49 (15)
C17—C16—C24	118.55 (13)	118.62 (13)	118.35 (15)	118.66 (15)	118.3 (2)	118.8 (2)	118.47 (14)	118.46 (14)
C17—C16—C8	120.31 (13)	120.94 (14)	120.34 (16)	120.74 (16)	120.7 (2)	120.5 (2)	120.75 (14)	120.70 (14)
C24—C16—C8	121.12 (13)	120.36 (13)	121.29 (14)	120.54 (15)	121.0 (2)	120.6 (2)	120.73 (13)	120.80 (13)
C16—C17—N4	124.73 (14)	124.63 (15)	124.92 (17)	124.61 (17)	125.4 (2)	124.6 (2)	124.94 (16)	124.91 (17)
N4—C18—C19	124.16 (14)	124.69 (14)	124.50 (16)	124.86 (16)	124.9 (2)	125.0 (2)	124.70 (15)	124.80 (15)
C20—C19—C24	119.72 (14)	119.71 (15)	119.84 (16)	119.55 (17)	119.5 (2)	119.5 (2)	119.57 (16)	119.41 (16)
C18—C19—C20	122.04 (14)	122.40 (14)	122.30 (16)	122.65 (17)	122.8 (2)	122.6 (2)	122.49 (15)	122.81 (16)
C18—C19—C24	118.24 (13)	117.90 (14)	117.86 (16)	117.80 (16)	117.7 (2)	117.9 (2)	117.94 (15)	117.78 (15)
C21—C20—C19	120.02 (15)	120.29 (15)	120.14 (17)	120.58 (18)	120.2 (2)	120.3 (2)	120.47 (17)	120.78 (18)
C20—C21—C22	120.18 (15)	120.20 (15)	120.18 (18)	119.94 (19)	120.2 (2)	120.3 (3)	120.16 (18)	120.12 (18)
C23—C22—C21	121.00 (15)	120.97 (16)	120.75 (17)	121.05 (19)	121.2 (3)	120.7 (3)	120.69 (19)	120.65 (19)
C22—C23—C24	120.33 (15)	120.24 (15)	120.62 (17)	120.45 (18)	120.3 (2)	120.8 (2)	120.79 (16)	120.64 (17)
C23—C24—C19	118.72 (13)	118.58 (14)	118.44 (16)	118.42 (16)	118.5 (2)	118.4 (2)	118.31 (15)	118.37 (15)
C16—C24—C19	117.40 (13)	123.92 (13)	117.62 (15)	117.51 (15)	117.6 (2)	117.4 (2)	117.54 (14)	117.57 (14)
C23—C24—C16	123.88 (13)	117.48 (14)	123.93 (15)	124.06 (16)	123.8 (2)	124.1 (2)	124.14 (14)	124.06 (14)