

Table S1. Hydrogen bonds for **10** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...I(2)#3	0.91	3.06	3.801(8)	140
N(1)-H(1B)...I(3)#3	0.91	3.06	3.750(7)	134
N(1)-H(1C)...I(1)#4	0.91	3.09	3.639(7)	120
N(2)-H(2A)...I(2)#6	0.91	3.04	3.583(7)	120
N(2)-H(2B)...I(5)#7	0.91	3.04	3.783(7)	140
N(2)-H(2C)...I(6)#8	0.91	2.66	3.559(8)	169
N(3A)-H(3A1)...I(1)#9	0.91	2.90	3.72(4)	150
N(3A)-H(3A3)...I(6)#9	0.91	2.78	3.55(5)	143
N(4A)-H(4A1)...I(5)#5	0.91	2.74	3.56(2)	151
N(4A)-H(4A2)...I(2)#5	0.91	3.13	3.75(2)	127
N(4A)-H(4A3)...I(6)	0.91	2.91	3.38(2)	113
N(3B)-H(3B1)...I(1)#9	0.91	2.70	3.52(4)	150
N(3B)-H(3B3)...I(6)#9	0.91	2.81	3.67(5)	158
N(4B)-H(4B1)...I(5)#5	0.91	2.96	3.745(17)	145
N(4B)-H(4B2)...I(6)	0.91	2.93	3.682(16)	142
N(4B)-H(4B3)...I(6)#5	0.91	2.84	3.320(13)	114

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+5/2 #2 -x+1,y-1/2,-z+5/2 #3 x,-y+3/2,z-1/2

#4 -x+1,-y+2,-z+2 #5 -x+1,-y+1,-z+2 #6 -x,-y+1,-z+2

#7 -x,-y+2,-z+2 #8 x-1,y,z #9 -x+2,-y+1,-z+2

#10 -x+2,-y,-z+2