Exploring conformationally flexible hydrogen-bond-functionalized ligand and counter anions in metal-organic frameworks of Cu(II)

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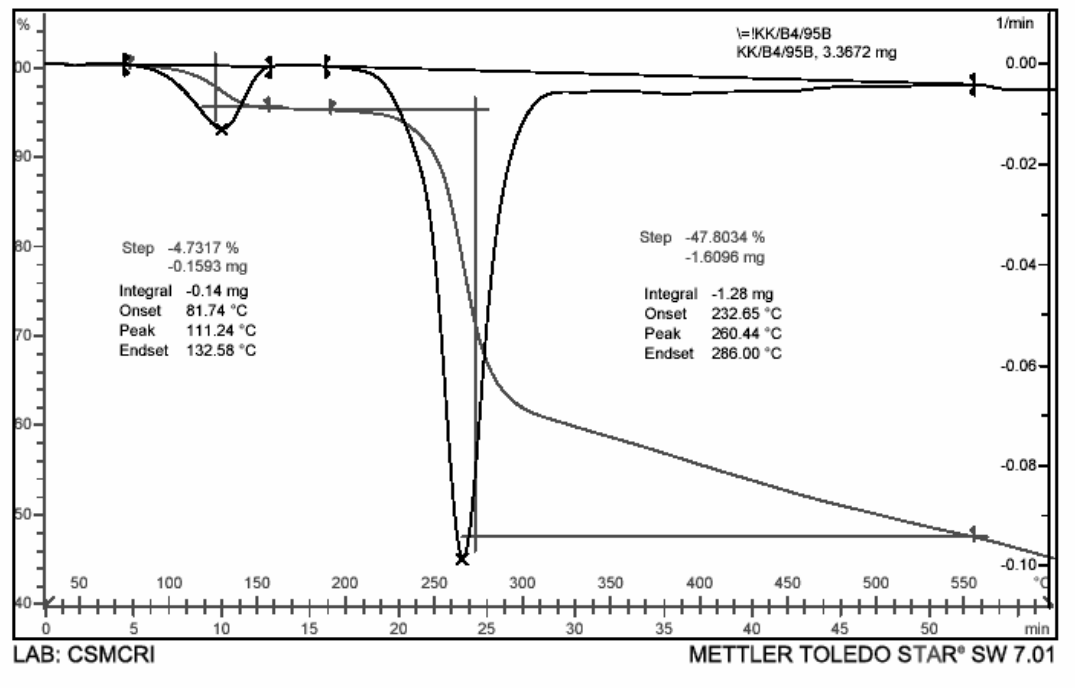
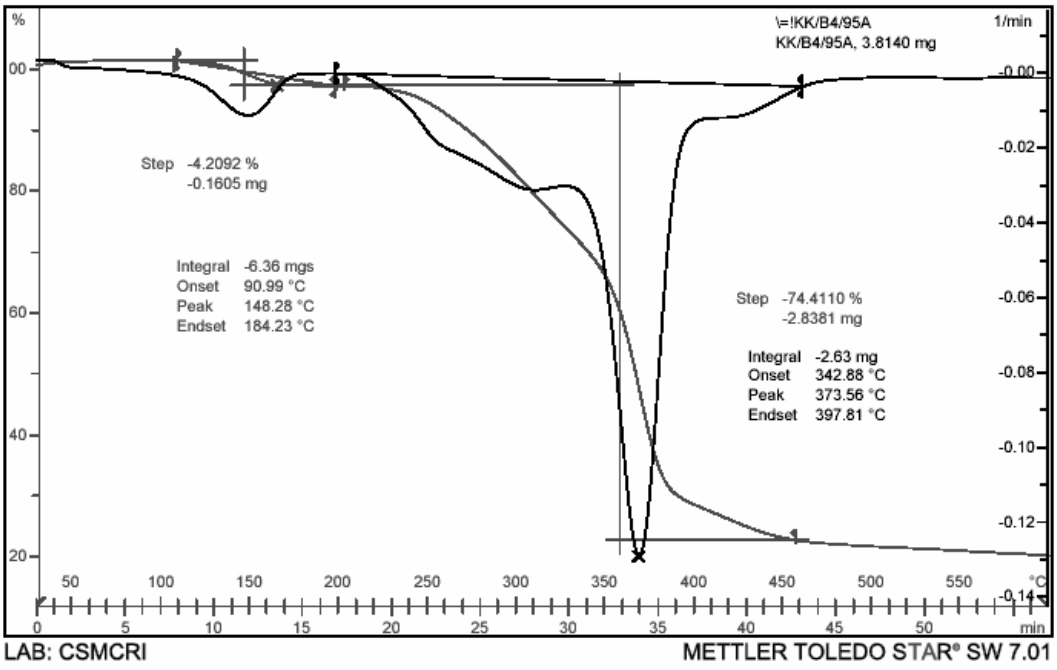
Thermal Analyses Plots

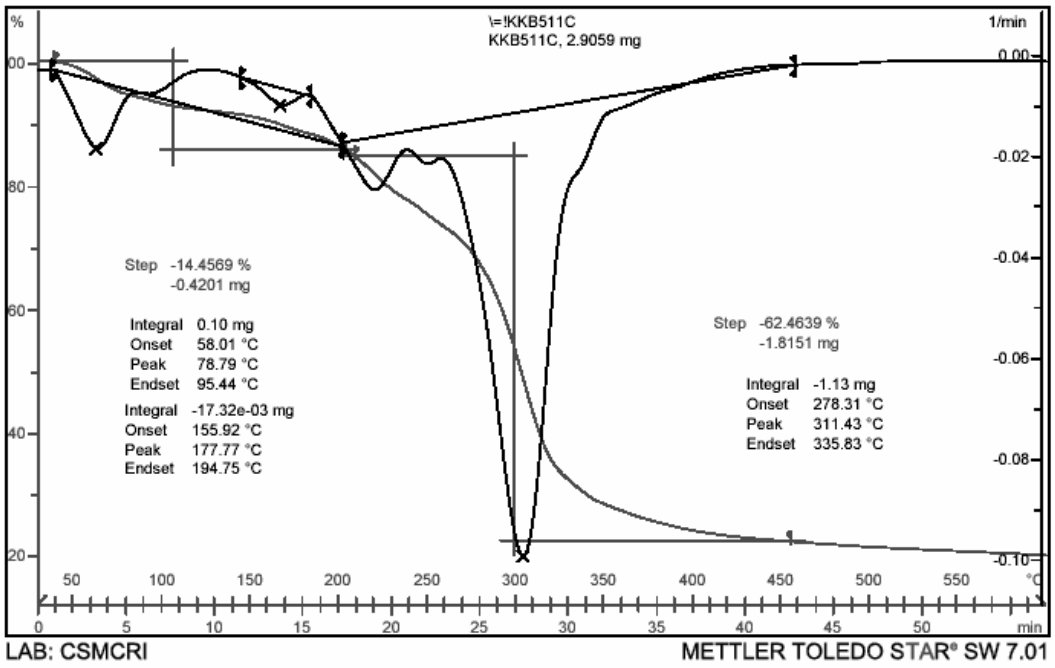
Compound 1



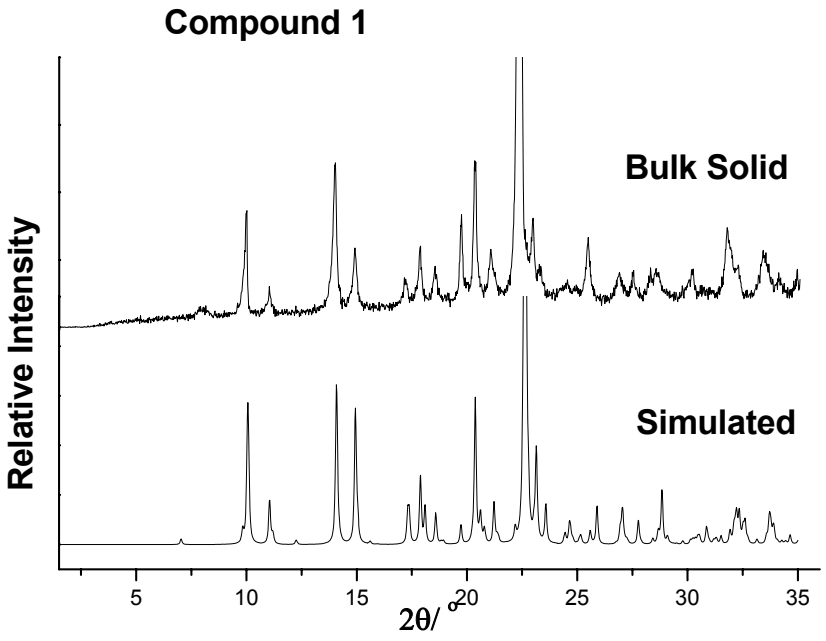
Compound 2

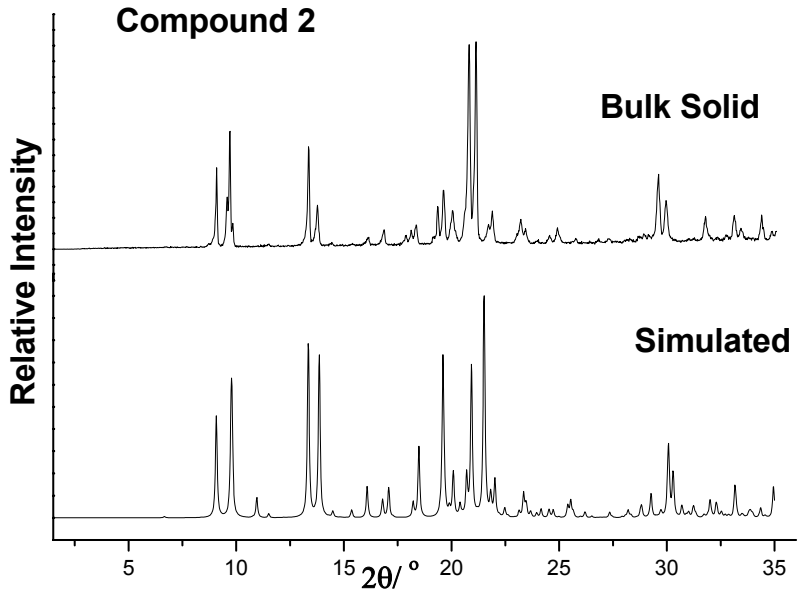


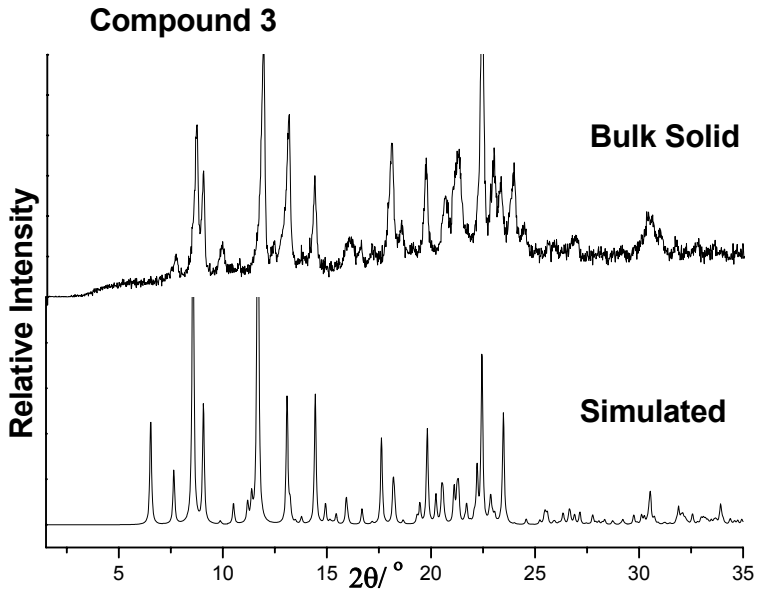
Compound 4

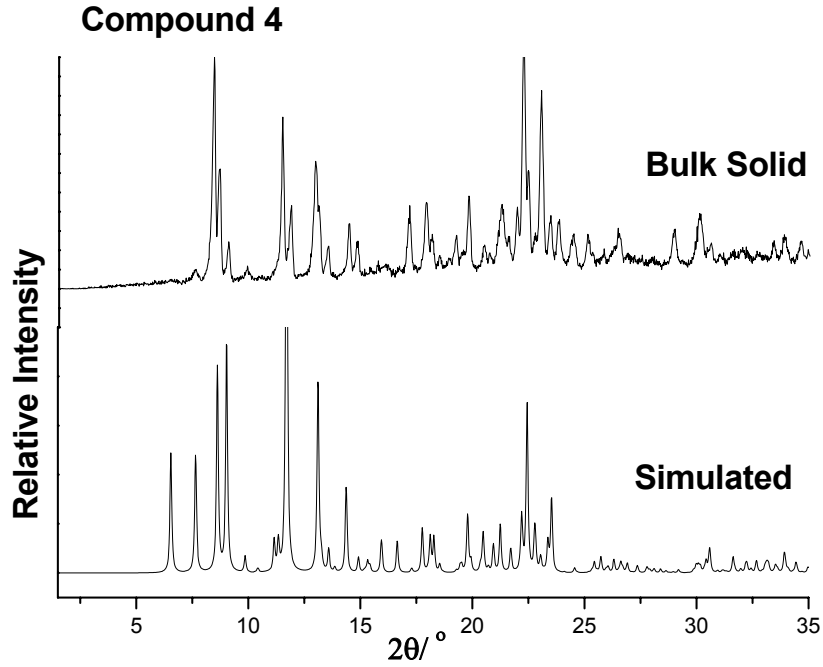


XRPD Patterns









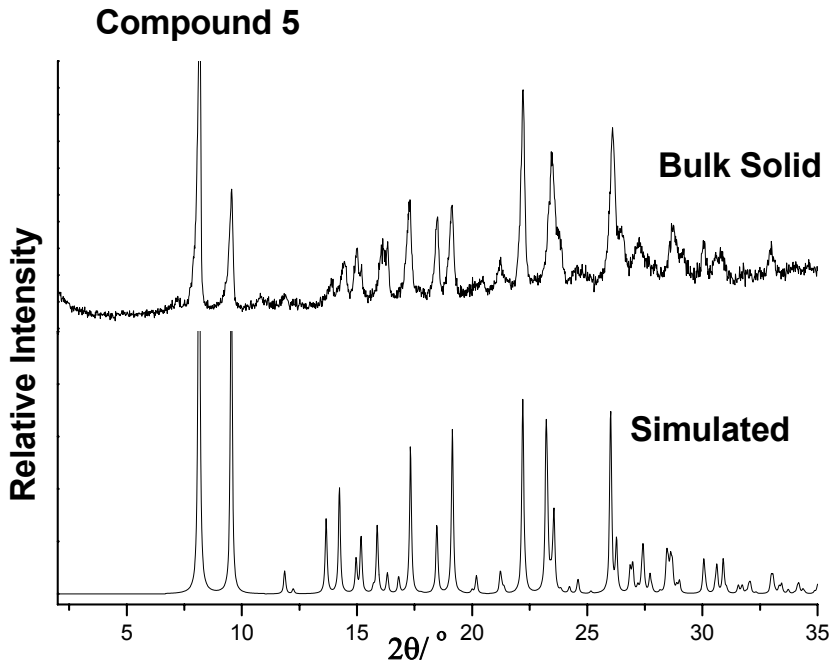


Table S1: Hydrogen bonding parameters for **1-6**

1					
D–H···A	**D–H/Å**	**H···A/Å**	**D···A/Å**	**D–H···A/^{0}**	**Symmetry operation for A**
N(7)–H(7)···O(41)	0.86	2.18	2.941(3)	148	x, y, z
N(10)–H(10)···O(41)	0.86	2.10	2.922(3)	159	x, y, z
N(23)–H(23)···O(37)	0.86	2.08	2.884(3)	155	x, y, z
N(26)–H(26)···O(35)	0.86	2.19	3.028(3)	164	x, y, z
O(43)–H(43A)···O(34)	0.84(3)	1.99(3)	2.806(3)	166(3)	x, y, z
O(43)–H(43B)···O(42)	0.82	2.12	2.821(3)	144	x, y, z
O(44)–H(44A)···O(9)	0.80(4)	2.17(4)	2.899(3)	153(3)	x, y, z
O(44)–H(44B)···O(37)	0.85(4)	2.11(4)	2.931(3)	164(3)	1+x, y, z
C(2)–H(2)···O(34)	0.93	2.58	3.505(3)	174	x, y, z
C(6)–H(6)···O(44)	0.93	2.40	3.138(3)	136	x, y, z
C(12)–H(12)···O(40)	0.93	2.52	3.380(4)	154	x, y, z
C(13)–H(13)···O(36)	0.93	2.48	3.325(3)	152	-x, 1/2+y, 3/2-z
C(14)–H(14)···O(44)	0.93	2.52	3.297(3)	142	-x, 1/2+y, 3/2-z
C(20)–H(20)···O(37)	0.93	2.54	3.291(3)	138	x, y, z
C(22)–H(22)···O(44)	0.93	2.45	3.282(3)	148	x, y, z
C(30)–H(30)···O(44)	0.93	2.42	3.185(3)	139	1-x, 1/2+y, 3/2-z
2					
N(7)–H(7)···O(47)	0.86	2.08	2.876(3)	154	x, y, z
N(10)–H(10)···O(46)	0.86	2.13	2.934(3)	155	x, y, z
N(23)–H(23)···O(40)	0.86	2.09	2.939(3)	171	x, y, z
N(26)–H(26)···O(39)	0.86	2.08	2.907(3)	161	x, y, z
O(49)–H(49A)···O(48)	0.78(3)	2.04(3)	2.809(3)	168(3)	-1+x, y, z
O(49)–H(49B)···O(38)	0.80(3)	2.10(4)	2.884(3)	166(3)	1-x, 1-y, 1-z
O(50)–H(50A)···O(46)	0.75(4)	2.34(4)	2.986(3)	144(4)	-1+x, y, z
O(50)–H(50B)···O(9)	0.73(4)	2.27(4)	2.980(3)	165(4)	x, y, z
C(2)–H(2)···O(50)	0.93	2.55	3.290(3)	137	1-x, -1/2+y, 1/2-z
C(12)–H(12)···O(46)	0.93	2.50	3.253(3)	138	x, y, z
C(14)–H(14)···O(39)	0.93	2.44	3.270(3)	148	x, 3/2-y, -1/2+z
C(16)–H(16)···O(50)	0.93	2.44	3.040(4)	122	x, y, z
C(18)–H(18)···O(50)	0.93	2.43	3.159(4)	135	1-x, -1/2+y, 1/2-z
C(28)–H(28)···O(39)	0.93	2.53	3.273(3)	137	x, y, z
C(30)–H(30)···O(47)	0.93	2.48	3.184(3)	133	2-x, 1/2+y, 1/2-z
C(32)–H(32)···O(50)	0.93	2.38	3.145(3)	139	x, y, z
3					
N(7)–H(7)···F(39)	0.86	2.45	2.985(6)	121	x, y, z
N(7)–H(7)···F(41)	0.86	2.18	3.037(6)	175	x, y, z

N(10)–H(10)···F(36)	0.86	2.13	2.952(6)	160	x, y, z
N(10)–H(10)···F(39)	0.86	2.40	2.998(6)	127	x, y, z
N(23)–H(23)···F(37)	0.86	2.11	2.951(6)	167	1-x, y, 1/2-z
N(23)–H(23)···F(39)	0.86	2.38	2.981(6)	127	1-x, y, 1/2-z
N(26)–H(26)···F(38)	0.86	2.06	2.909(6)	170	1-x, y, 1/2-z
N(26)–H(26)···F(39)	0.86	2.54	3.109(6)	125	1-x, y, 1/2-z
O(33)–H(33A)···F(37)	0.94(7)	1.91(7)	2.826(6)	164(6)	1-x, 1-y, 1-z
O(33)–H(33A)···F(40)	0.94(7)	2.39(7)	3.032(5)	126(5)	1-x, 1-y, 1-z
O(33)–H(33B)···O(42)	0.95(4)	2.11(4)	2.919(8)	143(3)	x, y, z
O(34)–H(34A)···F(38)	0.87	2.48	3.162(5)	136	-1/2+x, 1/2-y, -1/2+z
O(34)–H(34A)···F(40)	0.87	2.23	3.032(5)	153	-1/2+x, 1/2-y, -1/2+z
O(34)–H(34B)···O(9)	0.70	2.45	2.925(6)	126	x, y, z
O(34)–H(34B)···O(25)	0.70	2.35	2.969(6)	147	x, y, z
C(2)–H(2)···O(34)	0.93	2.54	3.405(6)	154	x, y, z
C(14)–H(14)···F(38)	0.93	2.55	3.181(6)	126	1-x, -y, 1-z
C(14)–H(14)···O(34)	0.93	2.57	3.446(7)	158	1/2-x, -1/2+y, 1/2-z
C(15)–H(15)···F(36)	0.93	2.50	3.388(6)	160	1-x, -y, 1-z
C(18)–H(18)···O(34)	0.93	2.59	3.449(7)	154'	x, y, z
C(22)–H(22)···O(42)	0.93	2.48	3.386(9)	165	x, y, z
C(30)–H(30)···O(34)	0.93	2.37	3.248(7)	158	1/2-x, -1/2+y, 1/2-z
4					
N(7)–H(7)···F(36)	0.86	2.01	2.855(4)	167	x, y, z
N(7)–H(7)···F(37)	0.86	2.54	3.082(4)	122	x, y, z
N(10)–H(10)···F(35)	0.86	2.07	2.923(4)	170	x, y, z
N(10)–H(10)···F(37)	0.86	2.42	2.992(4)	124	x, y, z
N(23)–H(23)···F(37)	0.86	2.27	2.960(4)	138	1-x, y, 3/2-z
N(23)–H(23)···F(38)	0.86	2.19	2.991(4)	156	1-x, y, 3/2-z
N(26)–H(26)···F(37)	0.86	2.37	2.969(4)	127	1-x, y, 3/2-z
N(26)–H(26)···F(39)	0.86	2.23	3.079(4)	167	1-x, y, 3/2-z
O(33)–H(33)···F(35)	0.82	2.00	2.823(3)	179	1/2-x, 1/2-y, 1-z
O(41)–H(41A)···O(9)	0.76	2.40	2.974(3)	133	x, y, z
O(41)–H(41A)···O(25)	0.76	2.30	2.894(4)	135	x, y, z
O(41)–H(41B)···F(40)	0.78	2.22	2.978(3)	165	1/2-x, 1/2-y, 1-z
C(6)–H(6)···O(41)	0.93	2.39	3.260(4)	156	1/2-x, -1/2+y, 3/2-z
C(12)–H(12)···O(41)	0.93	2.58	3.430(4)	153	x, y, z
C(21)–H(21)···F(38)	0.93	2.51	3.399(4)	159	x, -y, 1/2+z
C(22)–H(22)···O(41)	0.93	2.52	3.400(4)	158	1/2-x, -1/2+y, 3/2-z
C(28)–H(28)···O(41)	0.93	2.57	3.428(4)	153	x, y, z
5					
N(7)–H(7)···O(23)	0.86	1.98	2.836(4)	179	2-x, -y, 1-z
N(10)–H(10)···O(21)	0.86	2.26	3.012(5)	146	2-x, -y, 1-z
O(17)–H(17A)···O(24)	0.82	2.05	2.870(5)	177	x, 1/2-y, -1/2+z

O(17)–H(17B)···O(23)	0.86(5)	1.91(5)	2.744(6)	163(3)	-1+x, y, z
O(18)–H(18A)···O(22)	0.82	1.95	2.774(5)	179	x, 1/2-y, 1/2+z
O(18)–H(18B)···O(24)	0.85(7)	1.94(7)	2.786(6)	173(7)	x, y, z
O(24)–H(24)···O(22)	0.82	2.01	2.822(5)	172	-1+x, y, z
C(16)–H(16)···O(21)	0.93	2.51	3.321(6)	145	2-x, -y, 1-z
6					
N(7)–H(7)···O(27)	0.88	1.98	2.845(3)	166	x, y, -1+z
N(10)–H(10)···O(26)	0.88	2.06	2.928(3)	170	x, y, -1+z
O(21)–H(21)···O(26)	0.84	2.47	3.030(3)	125	1+x, y, -1+z
O(21)–H(21B)···O(24)	0.88(2)	2.12(2)	2.960(3)	159.2(16)	1-x, 1-y, 1-z
O(21)–H(21B)···O(27)	0.88(2)	2.222(19)	2.882(3)	131.4(18)	1-x, 1-y, 1-z
O(22)–H(22B)···O(19)	0.84	2.00	2.735(4)	145	-1+x, y, 1+z
O(23)–H(23B)···O(20)	0.97	2.16	2.943(3)	137	-1+x, y, 1+z
O(23)–H(23B)···O(26)	0.97	2.35	3.016(3)	125	x, y, z
C(12)–H(12)···O(20)	0.95	2.56	3.479(4)	162	-1+x, y, z