CHAPTER II

Hydrogen bonds for complex 3b-I·$CHCl_3$

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(22)-H(22B)...I(1)	0.99	3.01	3.863(5)	145.3
C(47)-H(47B)...O(1)#1	0.98	2.35	3.325(8)	173.7

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y+1/2,-z+1

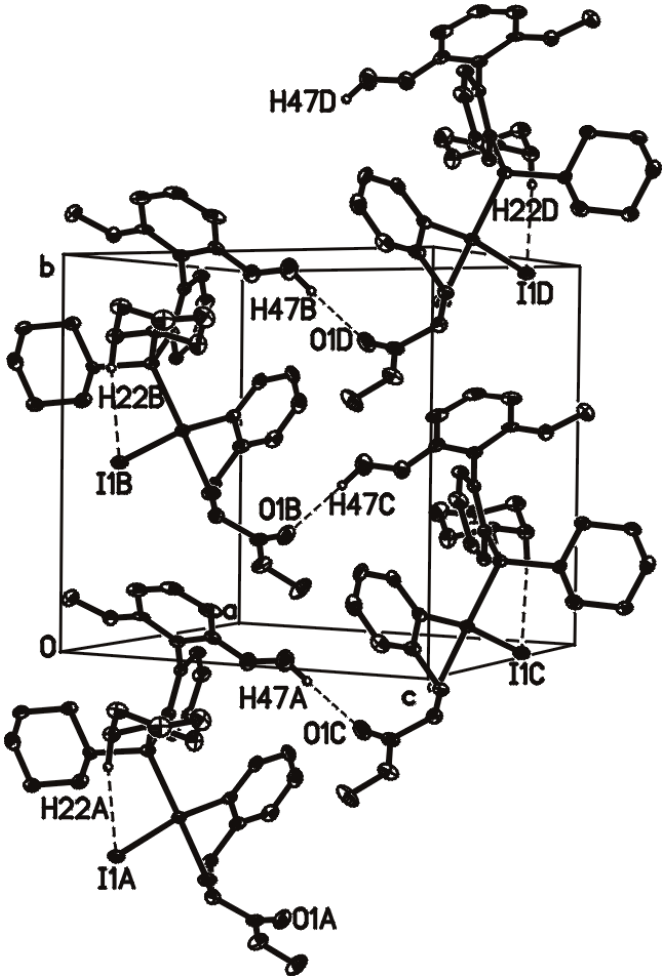

Figure. View of the hydrogen bond interactions in complex **3b-I**·$CHCl_3$. Only atoms involved in the H bonding are labeled.

CHAPTER III

Hydrogen bonds for complex Ia·2MeCN

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1B)...O(6)#1	0.82(3)	2.15(4)	2.875(5)	147(4)
O(1)-H(01)...O(4)#2	0.80(6)	1.92(6)	2.726(5)	176(6)
C(14)-H(14A)...O(5)	0.98	2.29	3.190(7)	152.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 x+1,y,z

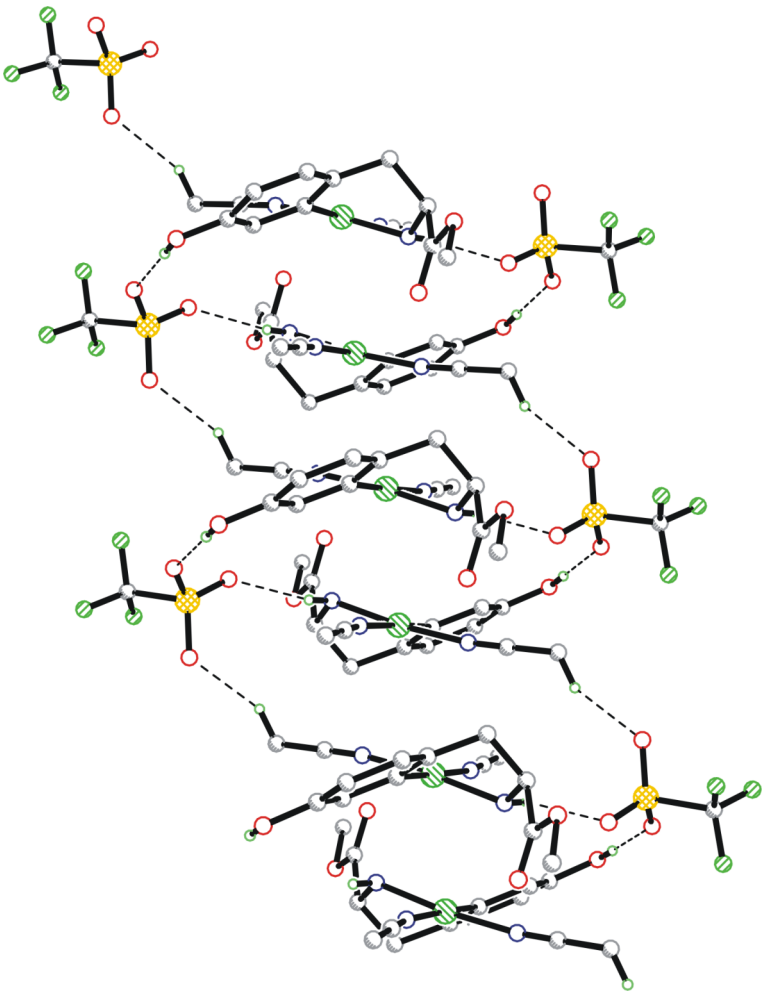

Figure. X-ray packing view of complex **Ia**·2MeCN showing the double chains along the *a* axis formed through hydrogen bond interactions.

Hydrogen bonds for complex 3a-OAc

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01B)...O(1)#1	0.831(15)	2.16(2)	2.885(3)	146(3)
O(1)-H(02)...O(5)#1	0.802(18)	1.842(19)	2.642(3)	175(4)
C(44)-H(44)...O(1)#2	0.95	2.50	3.394(4)	156.2

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2 #2 -x+1,-y,-z+2

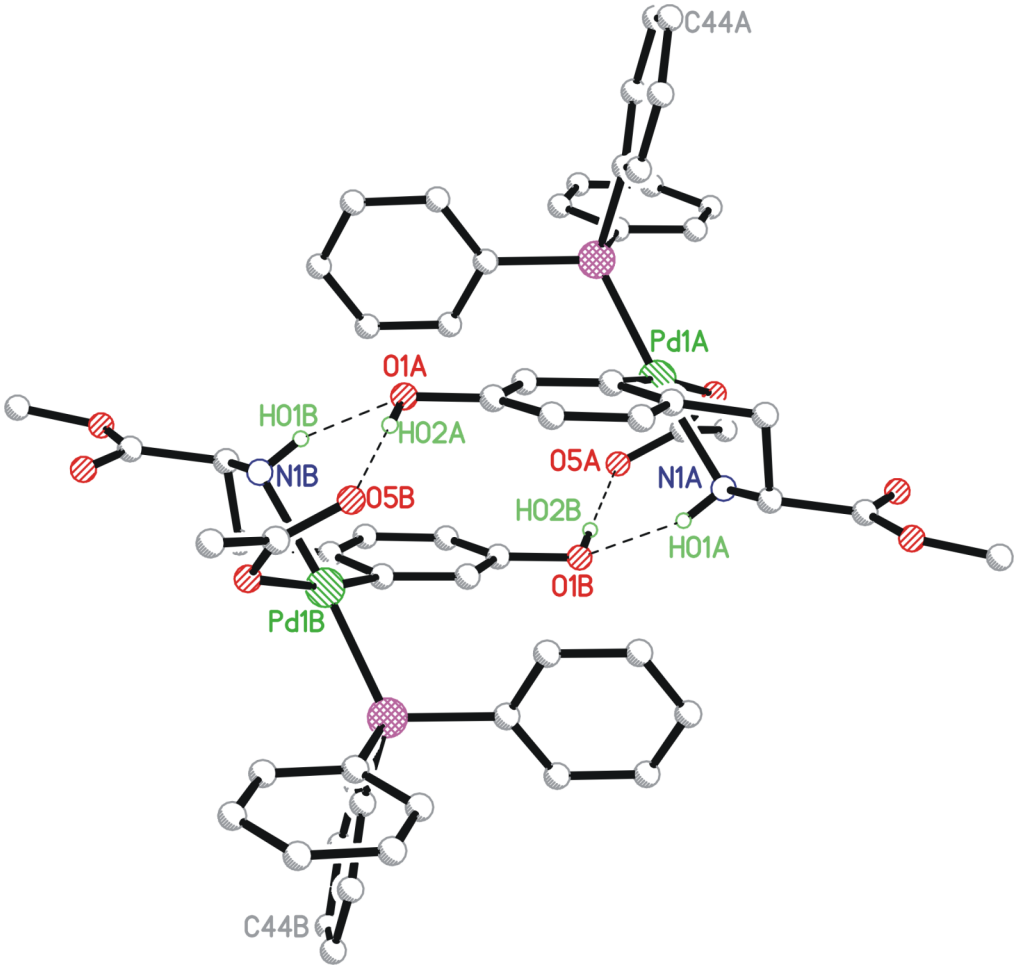

Figure. X-ray packing view of complex **3a-OAc** showing the dimers formed through hydrogen bond interactions involving the OH groups.

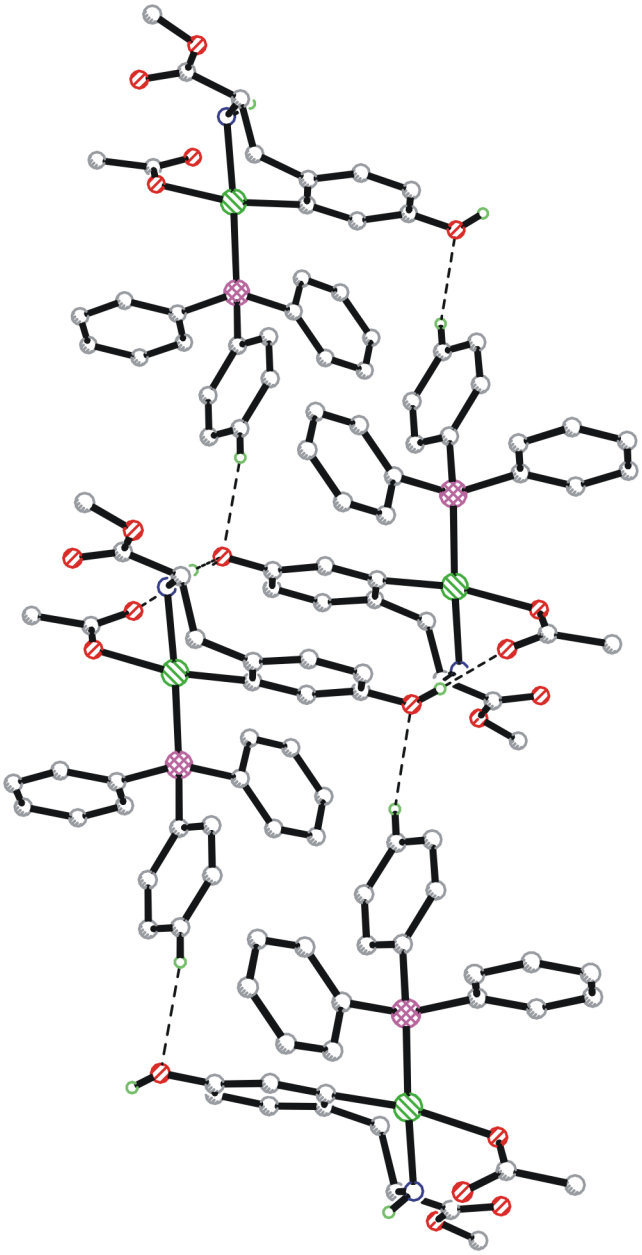

Figure. X-ray packing view of complex **3a-OAc** showing the double chains along the *b* axis formed through hydrogen bond interactions.

Hydrogen bonds for complex 6b-Br

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01B)...Br(2)#3	0.84(2)	2.76(2)	3.536(2)	155(3)
N(2)-H(02B)...Br(1)#4	0.83(2)	2.75(2)	3.549(3)	161(3)
C(30)-H(30B)...O(2)#5	0.98	2.51	3.288(4)	136.3

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z #2 -x+1,-y+1,-z #3 x,y+1,z #4 x-1,y,z #5 -x+2,-y+2,-z+1

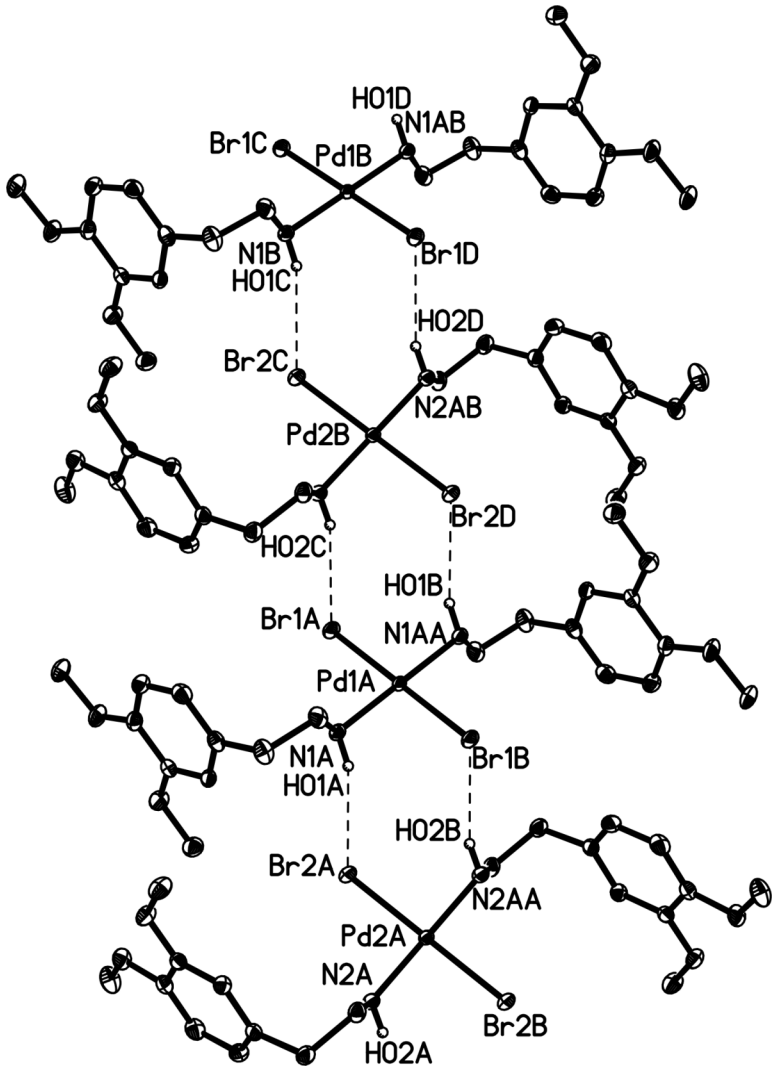

Figure. X-ray packing view of complex **6b-Br** showing the chains formed through N–H···Br hydrogen bond interactions.

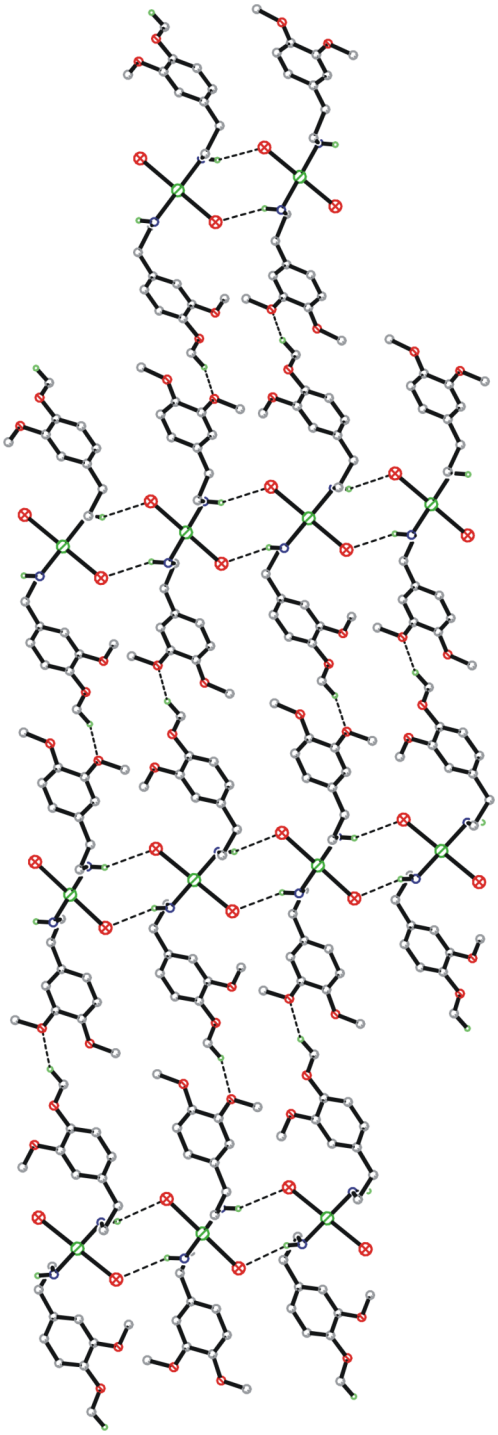

Figure. X-ray packing view of complex **6b-Br** showing the layers formed through hydrogen bond interactions.

Hydrogen bonds for complex 6b-OAc·H_2O

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01B)...O(99)	0.85(3)	2.03(3)	2.876(3)	172(2)
N(1)-H(01A)...O(1)#2	0.85(3)	2.25(3)	2.985(2)	146(2)
O(99)-H(09A)...O(2)#3	0.81(2)	2.00(2)	2.809(2)	175(3)
O(99)-H(09B)...O(2)#4	0.82(2)	2.00(2)	2.814(2)	172(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z #2 -x+1,-y+1,-z #3 -x+1,y+1/2,-z+1/2 #4 x,y+1,z

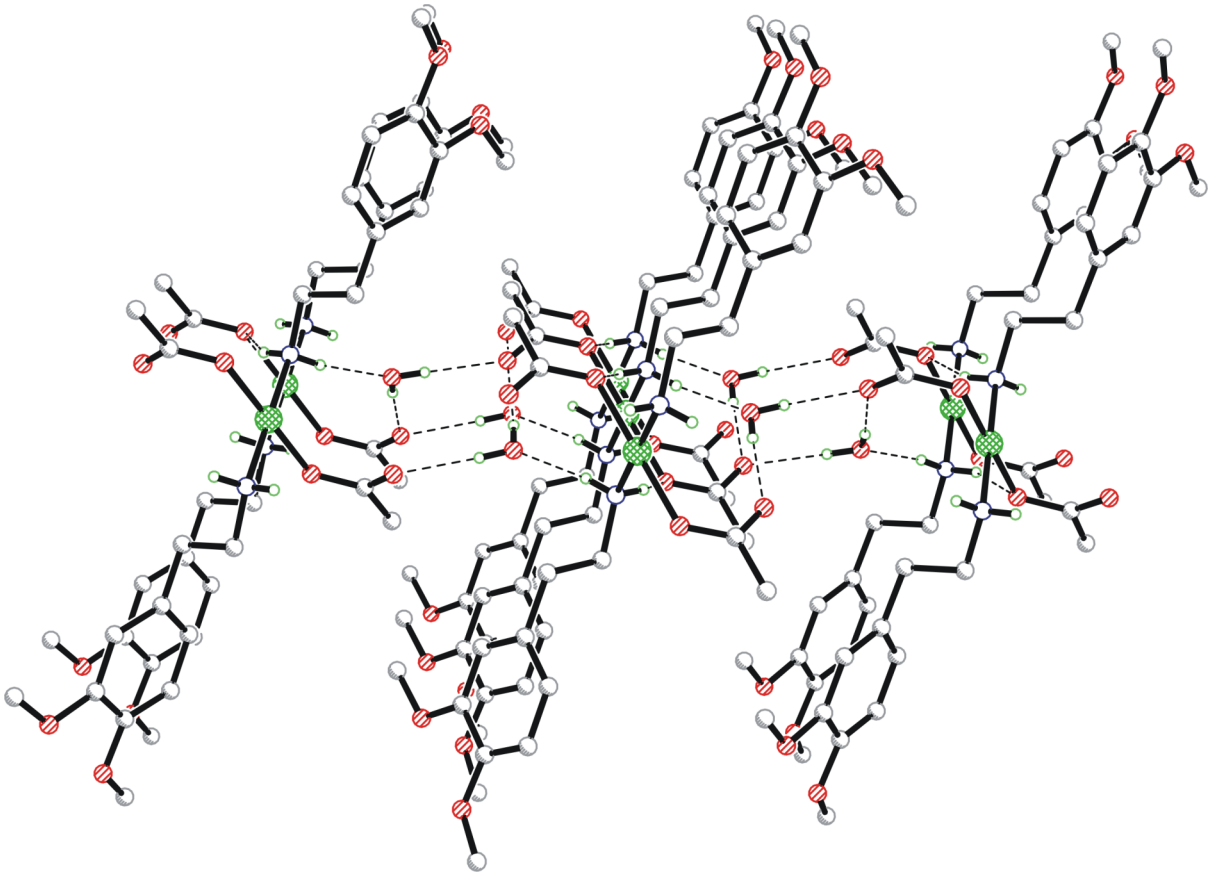

Figure. X-ray packing view of complex **6b-OAc**·H_2O showing the tridimensional net formed through hydrogen bond interactions.

Hydrogen bonds for complex 7b-OAc

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01B)...O(6)#1	0.810(16)	2.257(17)	2.9902(19)	150.8(18)
N(1)-H(01A)...O(4)#1	0.815(16)	2.127(16)	2.9375(18)	173.5(19)
C(44)-H(44)...O(4)#2	0.95	2.42	3.341(2)	164.2

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+2 #2 -x-1,-y,-z+2

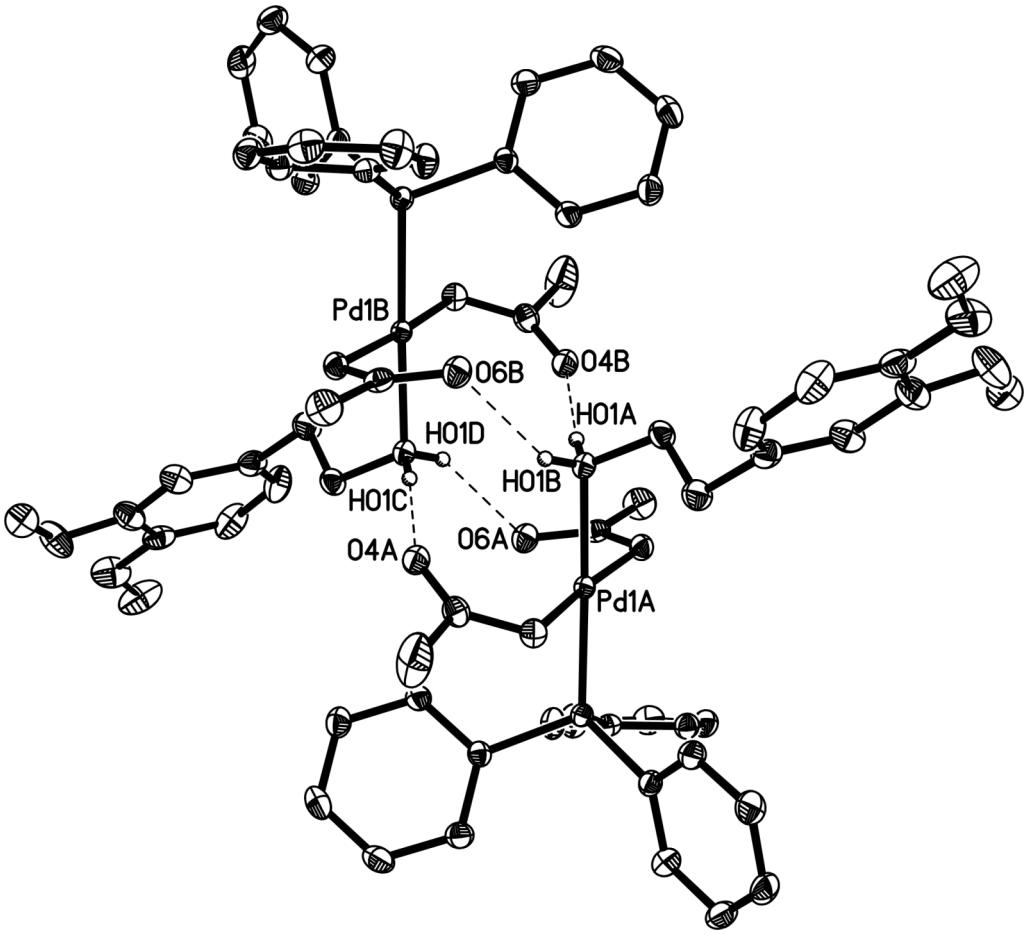

Figure. X-ray packing view of complex **7b-OAc** showing the dimers formed through N–H···O_{OAc} hydrogen bond interactions.

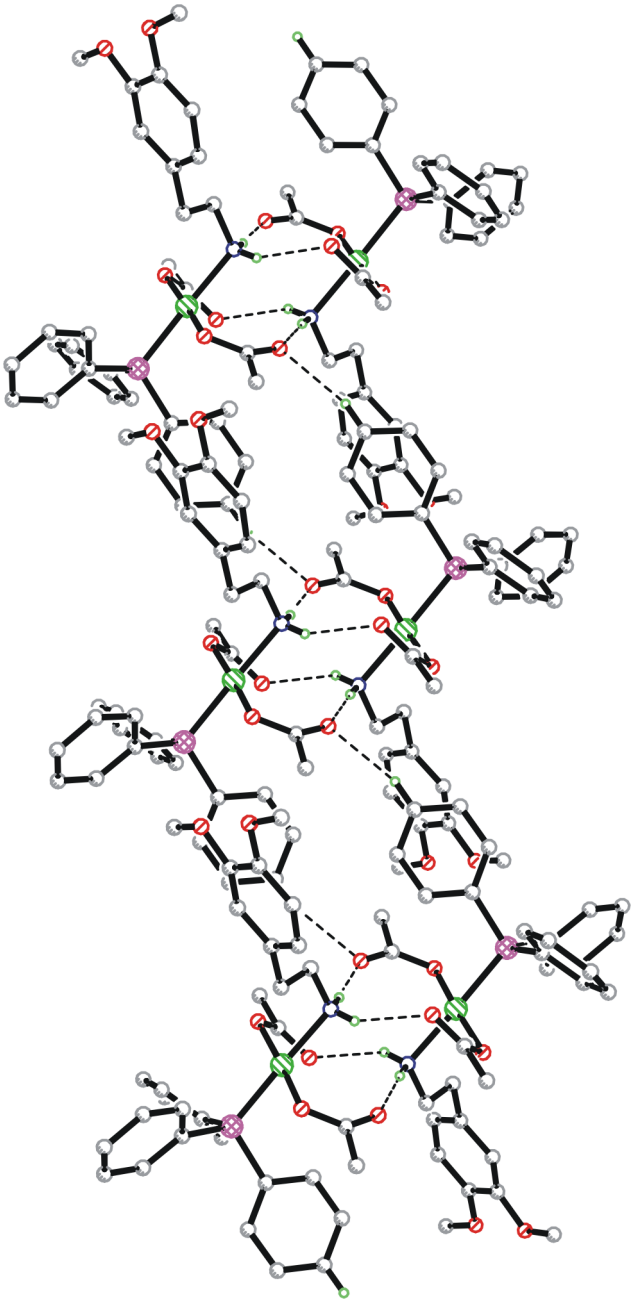

Figure. X-ray packing view of complex **7b-OAc** showing the double chains along the *a* axis formed through hydrogen bond interactions.

CHAPTER IV

Hydrogen bonds for complex 3a2

Table . Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01A)...O(3)	0.90(3)	2.21(3)	2.951(4)	140(3)
N(1)-H(01B)...O(3)#1	0.88(3)	2.28(3)	3.084(4)	152(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

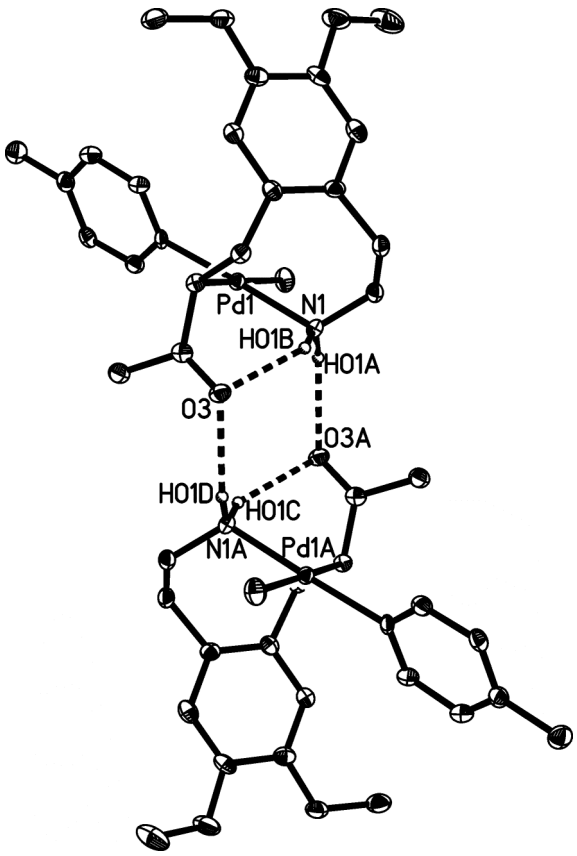

Figure. X-ray packing view of complex **3a2** showing the dimers formed through hydrogen bond interactions.

Hydrogen bonds for compound 4a1

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(03)...O(4)#1	0.824(18)	2.53(3)	3.199(3)	140(3)
N(3)-H(03)...O(5)#1	0.824(18)	2.30(2)	3.050(3)	152(3)
C(6)-H(6A)...O(1)#2	0.99	2.41	3.394(4)	171.8

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,-z #2 -x+2,y-1/2,-z+1/2

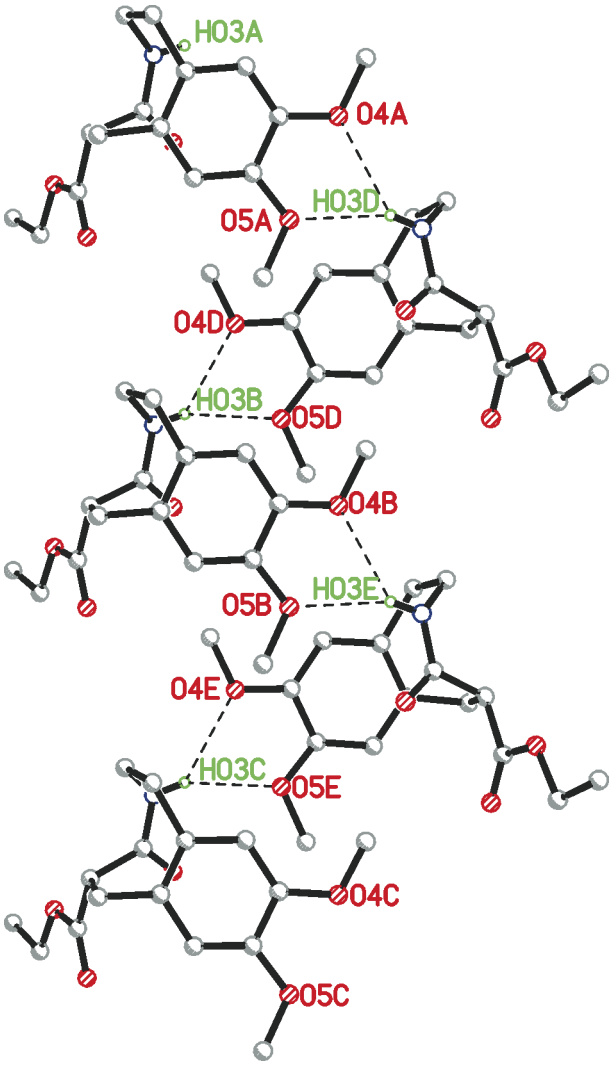

Figure. X-ray packing view of complex **4a1** showing the zigzag chains along the *a* axis formed through hydrogen bond interactions. Adjacents chains are connected through non-classical C–H···O hydrogen bonds to give a tridimentional net.

CHAPTER V

Hydrogen bonds for complex 5b·CH_2Cl_2

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(99)-H(99B)...Br(1)	0.99	2.89	3.766(3)	147.6
C(44)-H(44)...O(1)#1	0.95	2.52	3.319(3)	141.2
C(44)-H(44)...O(2)#1	0.95	2.58	3.440(3)	151.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+1

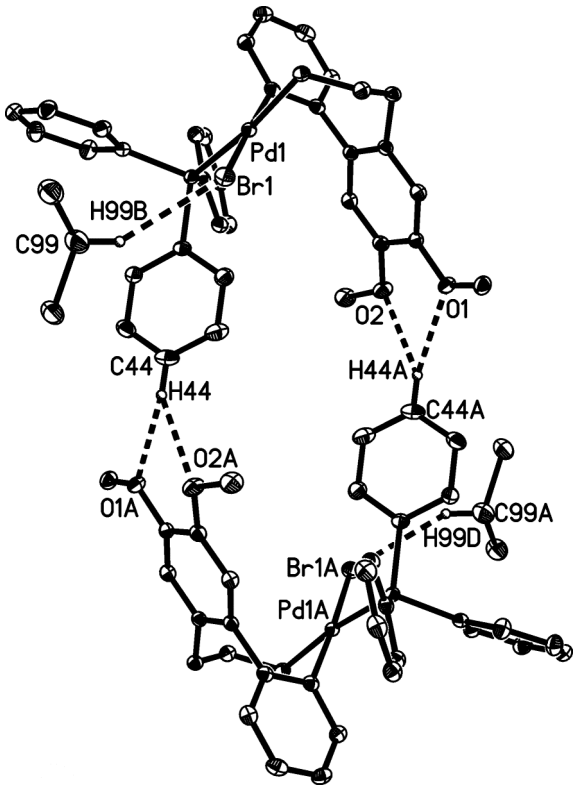

Figure. X-ray packing view of complex **5b**·CH_2Cl_2 (50% probability) showing the dimers formed through hydrogen bonds. Hydrogen interaction with the solvent is also shown.

Hydrogen bonds for complex 6b·2CH_2Cl_2

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	< (DHA)
C(11)–H(11B)···O(1)#2	0.98	2.44	3.358(5)	156.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+2 #2 -x+1,-y+1,-z+2

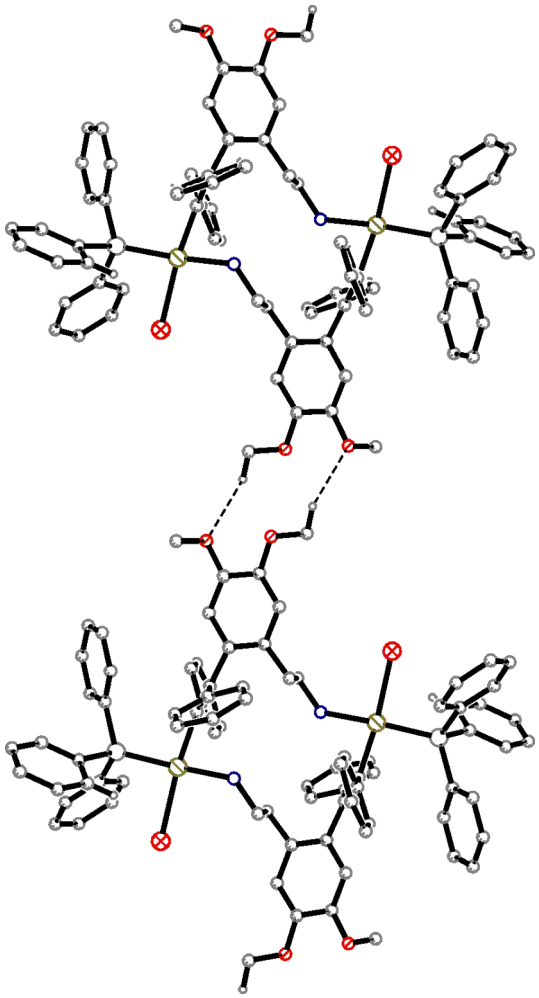

Figure. X-ray thermal ellipsoid plot (50% probability) of **6b**·2CH_2Cl_2 showing the chain along the *b* axis formed through hydrogen bond interactions.

Hydrogen bonds for complex 8b

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
C(13)-H(13)...O(2)#1	0.95	2.52	3.445(3)	165.4
C(28)-H(28B)...O(1)#2	0.98	2.60	3.535(2)	160.2

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z #2 -x+1,-y+1,-z

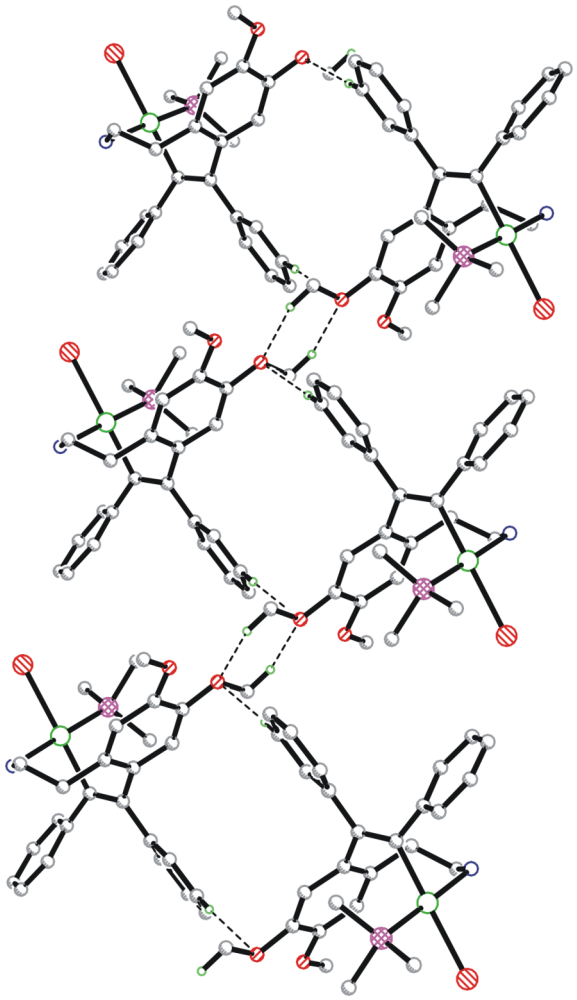

Figure. X-ray packing view (50% probability) of complex **8b** showing the double chains along the *b* axis formed through hydrogen bond interactions.

Hydrogen bonds for complex 11b

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(01A)...Br(1)#1	0.855(17)	2.791(19)	3.5413(16)	147.3(18)
C(17)-H(17A)...O(2)#2	0.98	2.60	3.493(3)	152.2

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z

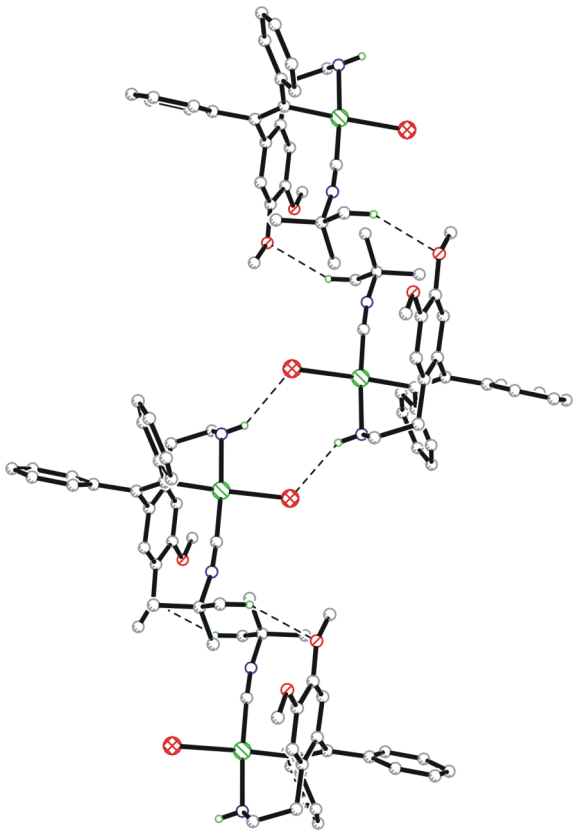

Figure. X-ray packing view (50% probability) of compound **11b** showing the zigzag chain along the direction (1 0 –1) formed through hydrogen bond interactions.

Hydrogen bonds for complex 12b·1/2Et_2O

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(01B)...O(4)#1	0.873(16)	2.43(2)	3.123(2)	136(2)
N(4)-H(04A)...O(90)	0.867(15)	2.483(17)	3.286(3)	154(2)
C(71)-H(71B)...O(1)#2	0.98	2.52	3.457(3)	158.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 x-1,y-1,z

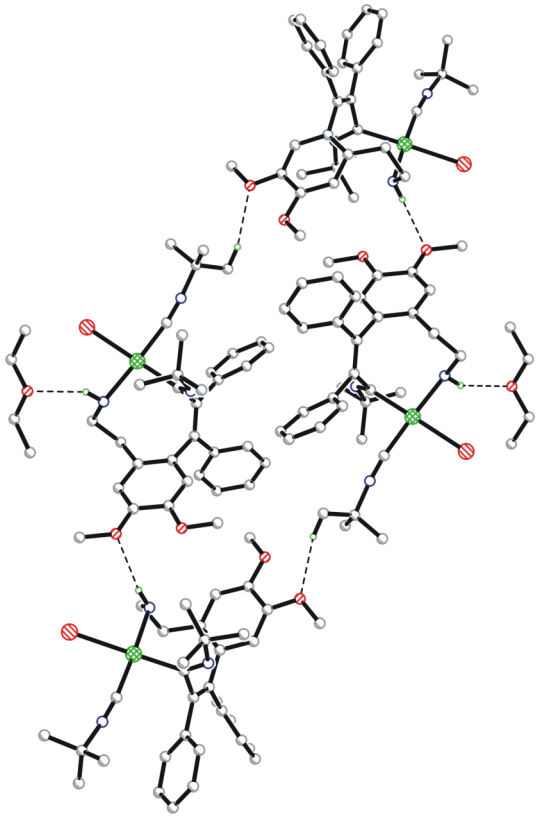

Figure. X-ray thermal ellipsoid plot (50% probability) of **12b**·1/2Et_2O showing the tetramer formed through hydrogen bond interactions.

Hydrogen bonds for complex 14b·$CHCl_3$·Et_2O

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01B)...O(81)#1	0.85(2)	2.38(3)	3.120(3)	146(3)
C(99)-H(99)...O(2)#2	1.00	2.28	3.193(3)	151.2

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 -x+1/2,-y+1,z+1/2

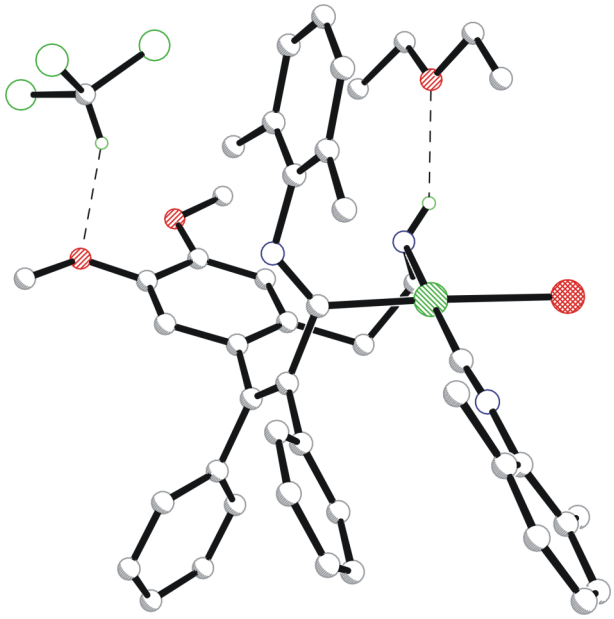

Figure. X-ray thermal ellipsoid plot (50% probability) of **14b**·$CHCl_3$·Et_2O showing the hidrogen bond interactions with the crystallization solvents.

Hydrogen bonds for compound 16b·Et_2O

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(01)...O(95)#1	0.86(2)	1.96(2)	2.7561(16)	153.2(18)
N(2)-H(02)...O(96)	0.845(18)	1.930(18)	2.7585(16)	166.5(16)
C(12)-H(12A)...F(3)	0.98	2.43	3.323(2)	151.5
C(12)-H(12C)...O(91)	0.98	2.59	3.463(2)	148.1
C(43)-H(43)...O(2)#2	0.95	2.45	3.3702(18)	163.1

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z #2 -x+1,-y+1,-z

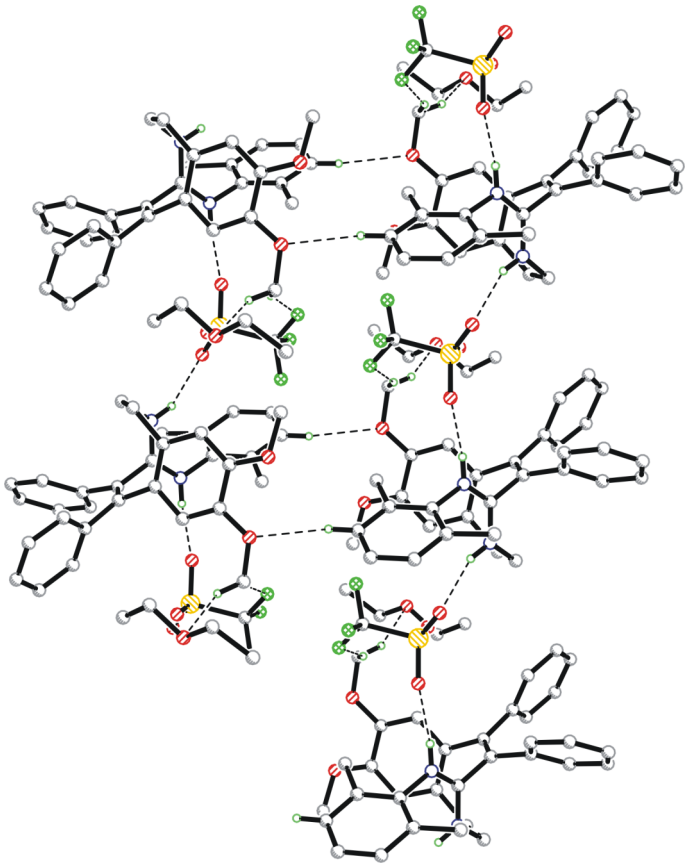

Figure. X-ray thermal ellipsoid plot (50% probability) of **16b**·Et_2O showing the layer parallel to the *ac* plane formed through hydrogen bond interactions.

Hydrogen bonds for compound 24b

Table. Hydrogen bonds (Å and deg).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...O(2)#1	0.94	2.50	3.381(3)	155.7
C(9)-H(9B)...O(1)#2	0.98	2.58	3.414(3)	142.7
N(1)-H(01)...O(1)#3	0.88(3)	2.07(3)	2.927(3)	162(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z+1/2 #2 x,y+1,z #3 -x,-y+1,-z

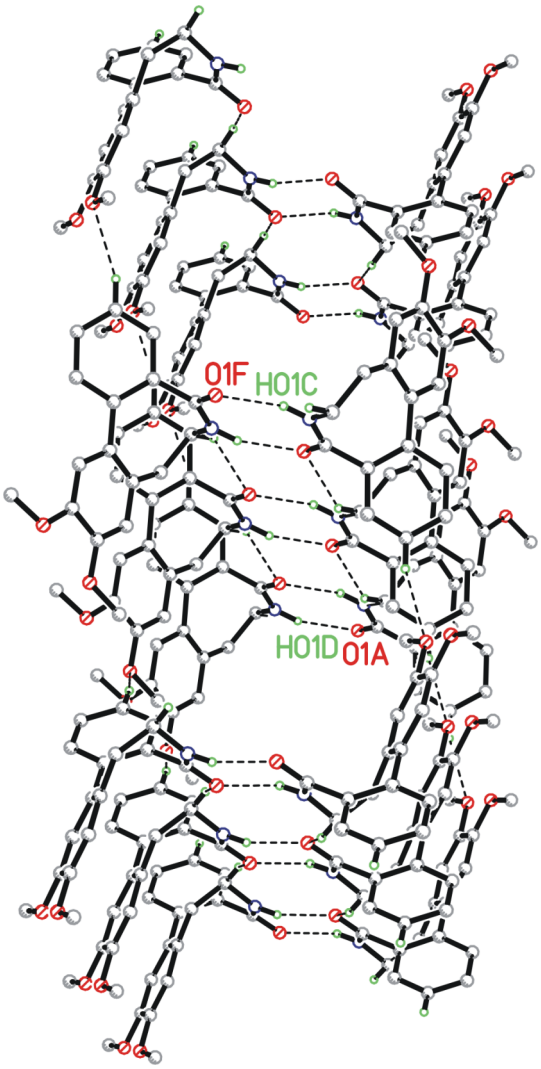

Figure. X-ray thermal ellipsoid plot (50% probability) of **16b**·Et_2O showing the double layers parallel to the *bc* plane formed through hydrogen bond interactions.

Hydrogen bonds for compound 25b

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(01A)...Br(1)#1	0.874(16)	2.372(17)	3.2338(17)	169(2)
N(1)-H(01B)...Br(2)#2	0.848(16)	2.412(17)	3.2568(17)	174(2)
N(1)-H(01C)...O(3)	0.863(17)	2.094(19)	2.882(2)	152(2)
C(13)-H(13B)...O(2)#3	0.98	2.59	3.538(2)	163.0
C(14)-H(14B)...Br(1)#4	0.98	2.82	3.7655(18)	162.9

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1 #2 x,y-1,z+1 #3 -x+2,-y+1,-z+2 #4 x+1,y+1,z+1

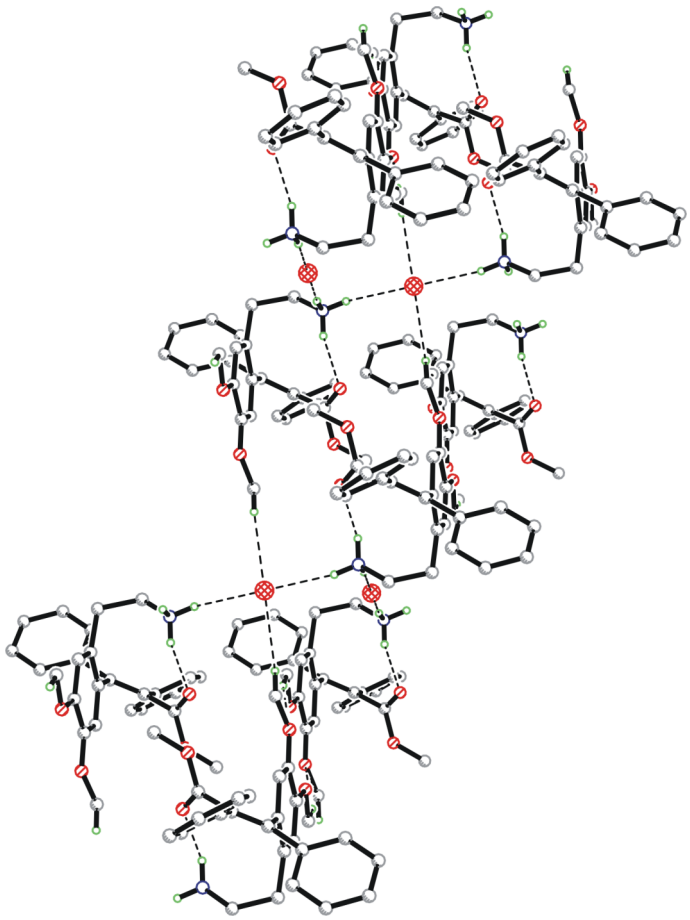

Figure. X-ray thermal ellipsoid plot (50% probability) of **25b** showing the double chain along the (1 1 0) direction formed through hydrogen bond interactions.

Hydrogen bonds for complex 32b

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
N(1)–H(01A)···Br(1)#1	0.84(4)	2.54(4)	3.364(4)	167(5)
C(24)–H(24)···Br(1)#2	0.95	2.82	3.692(5)	153.1

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2
#2 x,y+1,z

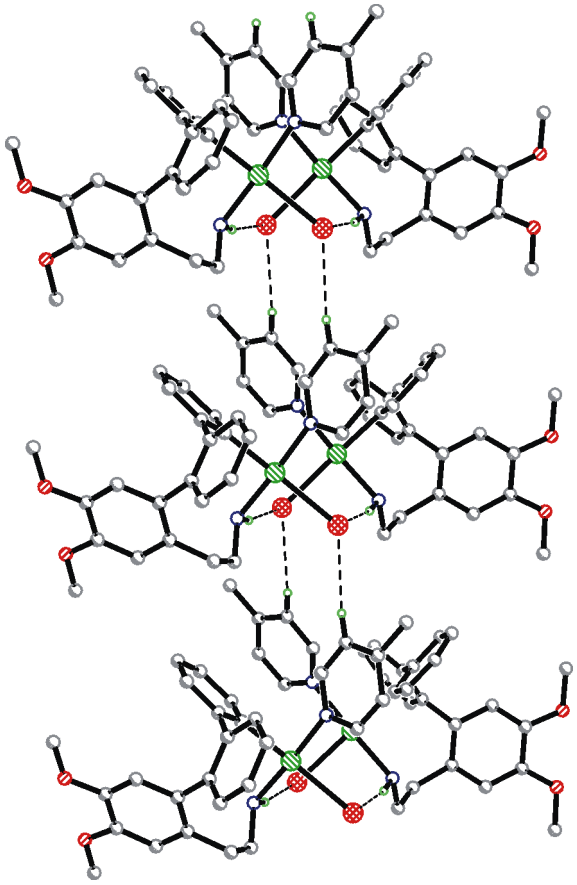

Figure. X-ray packing view of complex **32b** (50% probability) showing the double chain along the *b* axis formed through hydrogen bond interactions.

Hydrogen bonds for complex 35b·CH_2Cl_2

Table. Hydrogen bonds (Å and deg).

D–H···A	d(D–H)	d(H···A)	d(D···A)	< (DHA)
N(1)–H(01)···O(2)#1	0.84(3)	2.12(4)	2.927(3)	160(3)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,z

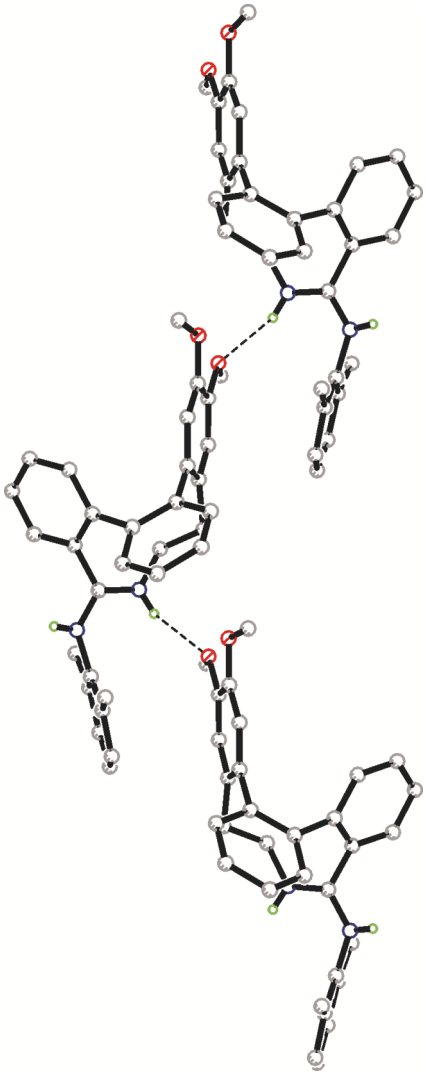

Figure. X-ray packing view of compound **35b**·CH_2Cl_2 showing the chain along the *a* axis formed through hydrogen bond interactions.