Supplementary Materials

Two-Dimensional Metal-Organic Frameworks (MOFs) Constructed from Heterotrinuclear Coordination Units and 4,4'-Biphenyldicarboxylate (BPDC) Ligands: $[Zn_2M(BPDC)_3(DMF)_2]\cdot 4DMF$ (M = Co^{II}, Ni^{II}, or Cd^{II}, DMF = *N,N'*-Dimethyl formamide)

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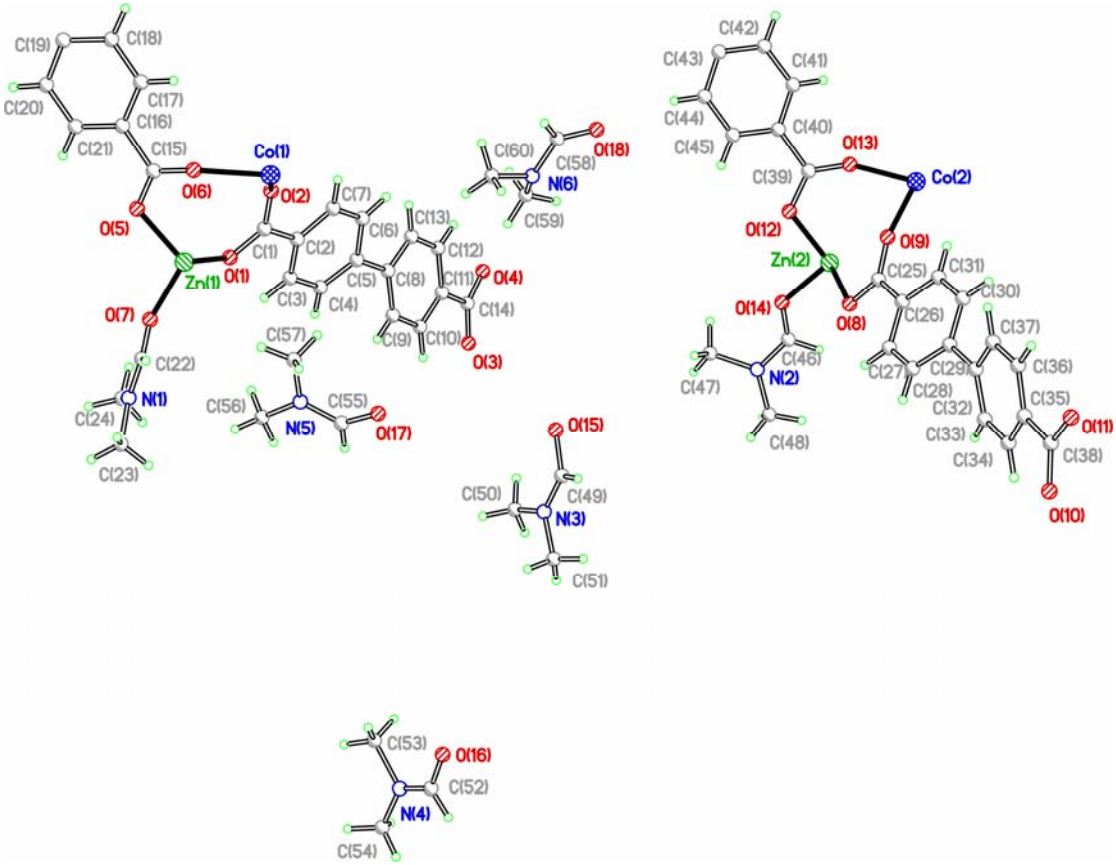

Fig. S1 Complete labelling scheme of compound **1**
(There are two independent Co atoms in compound 1, both of which lie on an inversion center)

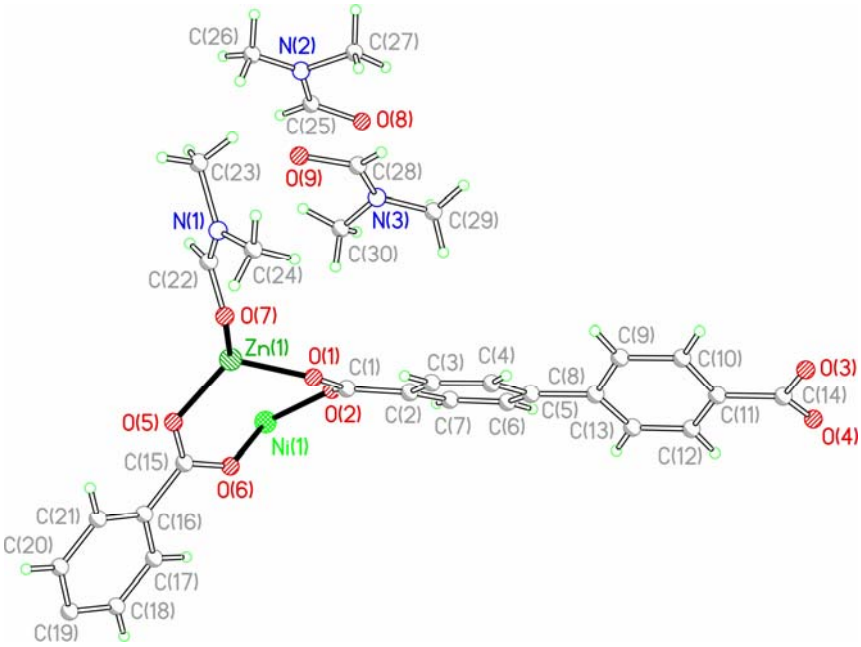

Fig. S2 Complete labelling scheme of compound **2**
(Ni(1) lies on an inversion centre. Compounds 2 and 3 are isomporphous and their structures have been refined with a common origin and identical labelling schemes.)

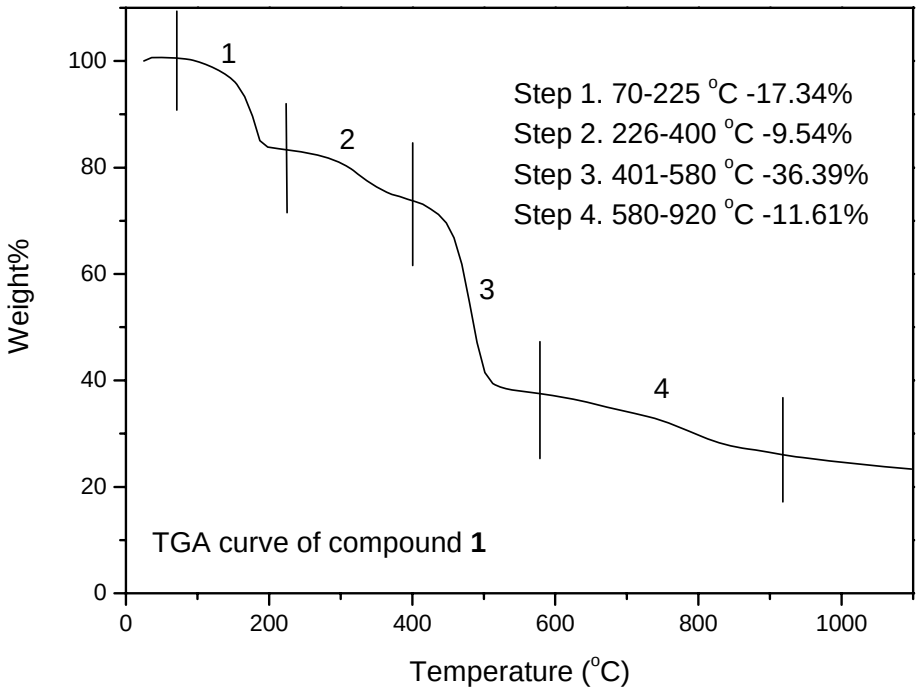

Fig. S3 Thermogravimetric analysis (TGA) curve of compound **1**.

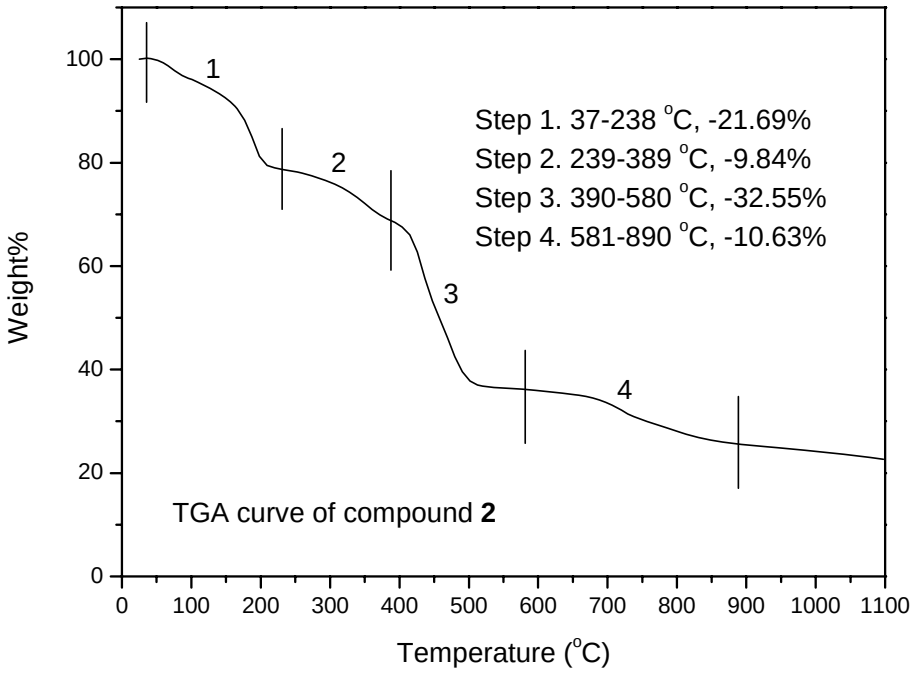

Fig. S4 TGA curve of compound **2**.

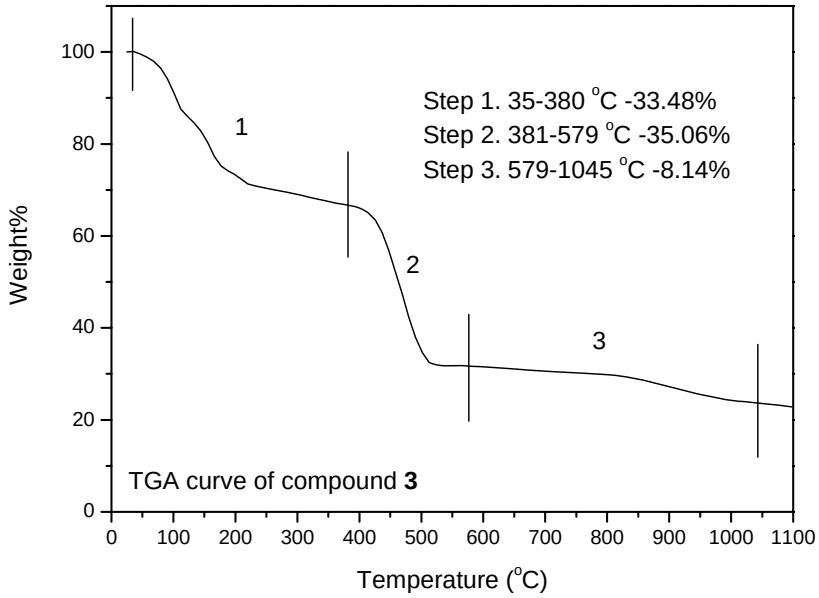

Fig. S5 TGA curve of compound **3**.

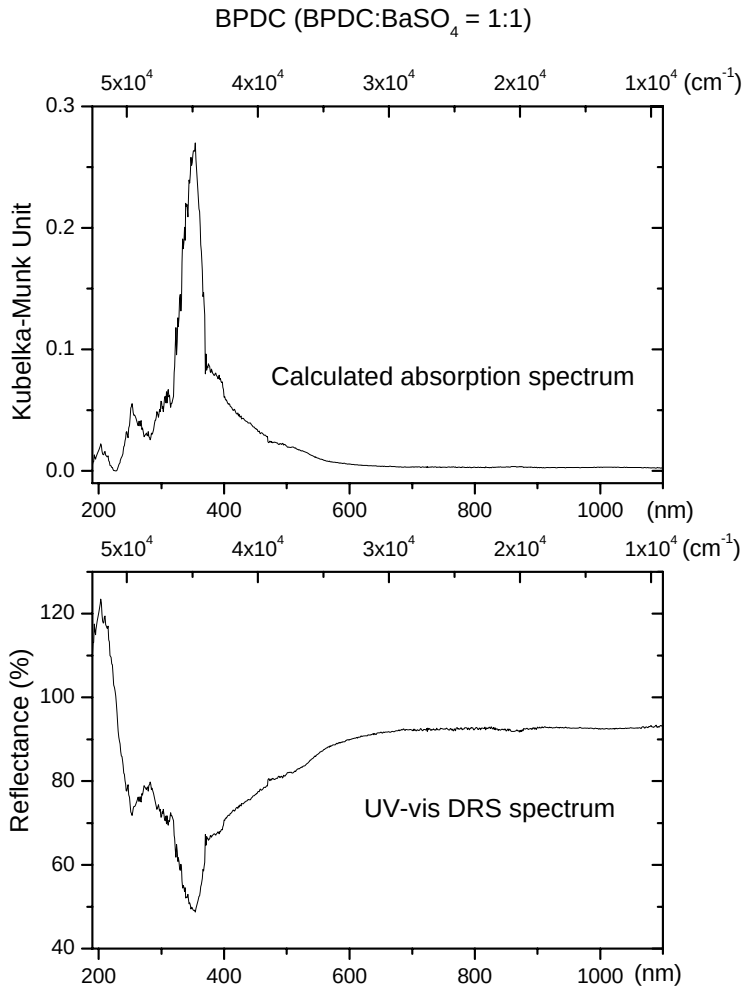

Fig. S6 UV-vis diffuse reflectance spectrum (DRS) (bottom) and calculated absorption spectrum (top) via the Kubelka-Munk function for the BPDC ligand (BPDC:$BaSO_4$ = 1:1).

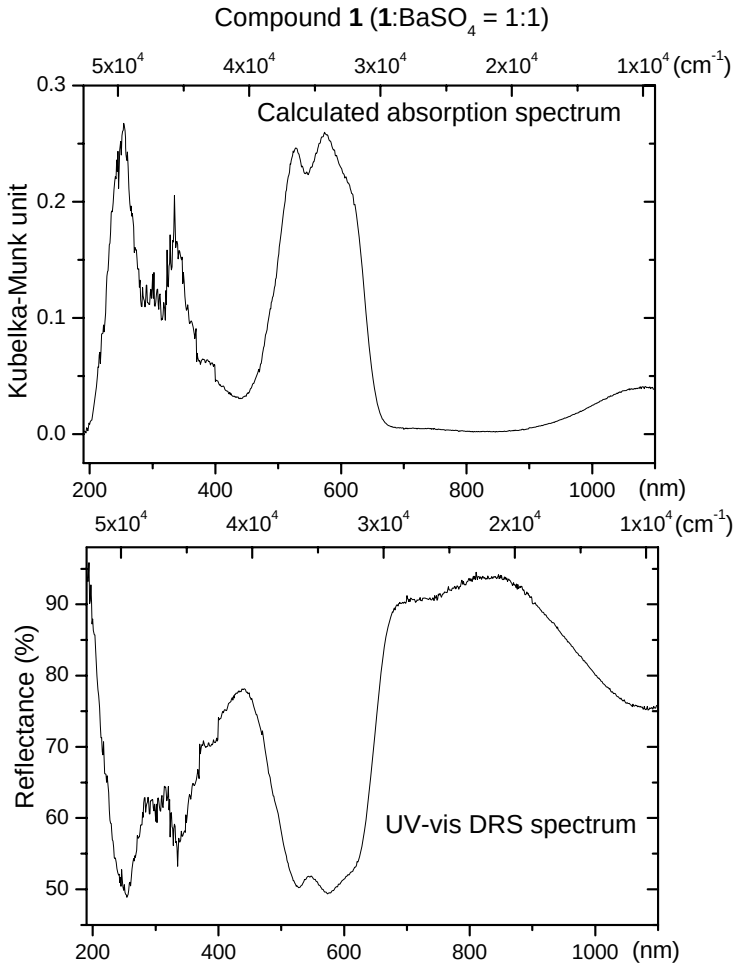

Fig. S7 UV-vis diffuse reflectance spectrum (DRS) (bottom) and calculated absorption spectrum (top) via the Kubelka-Munk function for Compound **1** (**1**:$BaSO_4$ = 1:1).

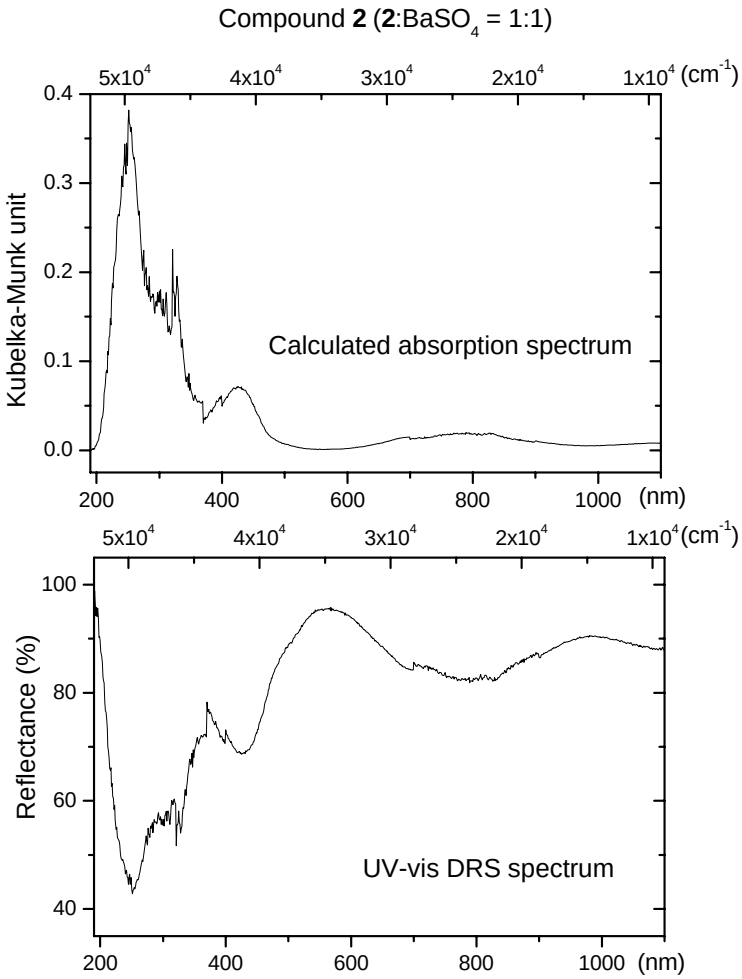

Fig. S8 UV-vis diffuse reflectance spectrum (DRS) (bottom) and calculated absorption spectrum (top) via the Kubelka-Munk function for Compound **2** (**2**:$BaSO_4$ = 1:1).

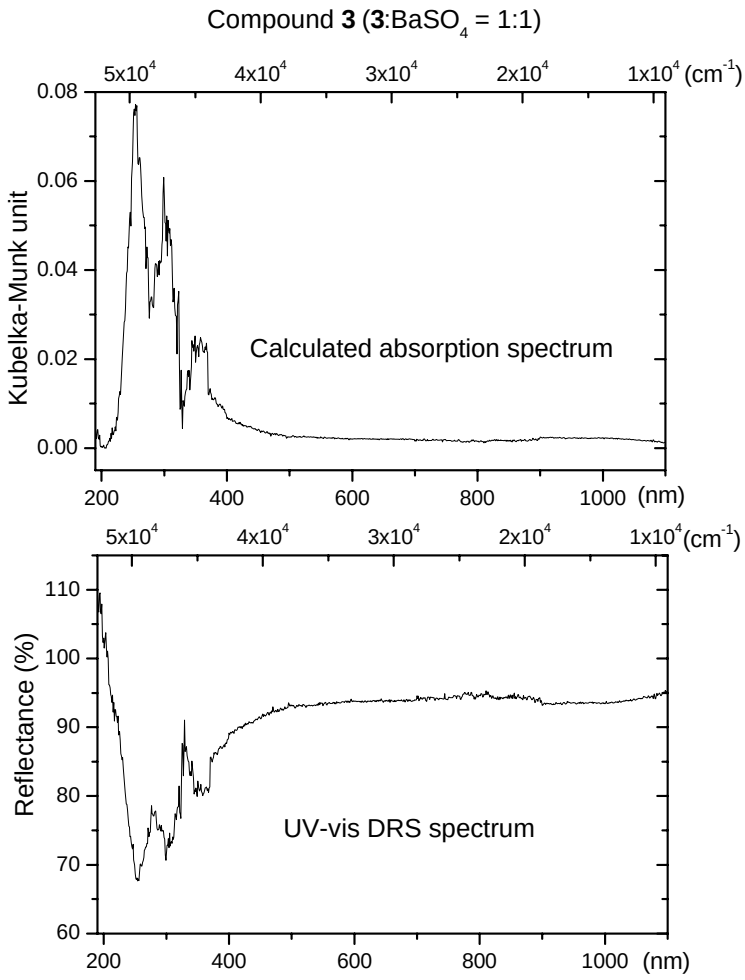

Fig. S9 UV-vis diffuse reflectance spectrum (DRS) (bottom) and calculated absorption spectrum (top) via the Kubelka-Munk function for Compound **3** (**3**:$BaSO_4$ = 1:1).

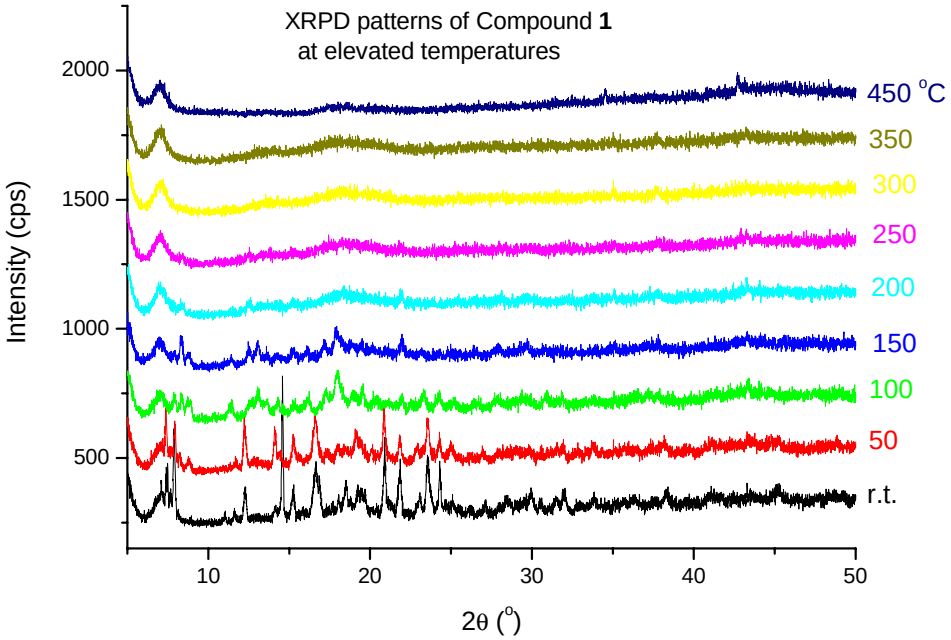

Fig. S10 X-ray Powder diffraction (XRPD) patterns of Compound **1** measured at elevated temperatures.

Table T1

Weak hydrogen-bonding parameters (Å and °) involving the occluded DMF molecules for 1-3

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Analysis of Potential Hydrogen Bonds and Schemes with
d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
==============================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above
(Possibly transformed, when MOVE .NE. 1.555)
==============================================================================================
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Compound 1

Nr	Typ	Res	Donor	---	H	....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	C(18)	--H(18)	..O(17)		[2555.05]	0.94	2.50	3.432(16)	173
2		1	C(20)	--H(20)	..O(17)		[4464.05]	0.94	2.34	3.270(15)	169
3		1	C(23)	--H(23B)	..O(16)		[3665.04]	0.97	2.56	3.41(2)	147
4	Intra	1	C(24)	--H(24C)	..O(7)		[ ]	0.97	2.35	2.761(12)	104
5		2	C(37)	--H(37)	..O(16)		[2655.04]	0.94	2.57	3.492(19)	166
6		2	C(44)	--H(44)	..O(18)		[2565.06]	0.94	2.47	3.40(2)	168
7		2	C(48)	--H(48A)	..O(15)		[2555.03]	0.97	2.37	3.29(3)	158
8	Intra	3	C(50)	--H(50A)	..O(15)		[ ]	0.97	2.27	2.74(4)	108
9		5	C(55)	--H(55)	..O(10)		[ ]	0.94	2.55	3.356(15)	143
10		6	C(59)	--H(59A)	..O(15)		[ ]	0.97	2.28	3.21(6)	163

```
:: No Classic Hydrogen Bonds Found

 Translation of ARU-code to Equivalent Position Code
=====================================================
   [  2555. ]  = 1/2-x,1/2+y,1/2-z
   [  4464. ]  = -1/2+x,3/2-y,-1/2+z
   [  3665. ]  = 1-x,1-y,-z
   [  2565. ]  = 1/2-x,3/2+y,1/2-z
   [  2655. ]  = 3/2-x,1/2+y,1/2-z
```

Compound 2

Nr	Typ	Res	Donor	---	H	....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	C(18)	--H(18)	..O(8)		[4565.02]	0.95	2.57	3.47(3)	158
2		1	C(20)	--H(20)	..O(8)		[2555.02]	0.95	2.46	3.34(3)	154
3	Intra	1	C(22)	--H(22)	..O(3)		[4455.01]	0.95	2.58	3.094(14)	114
4	Intra	2	C(27)	--H(27B)	..O(8)		[ ]	0.98	1.92	2.49(7)	114
5	Intra	3	C(30)	--H(30C)	..O(9)		[ ]	0.98	2.07	2.51(5)	105

```
:: No Classic Hydrogen Bonds Found

 Translation of ARU-code to Equivalent Position Code
=====================================================
   [  4455. ]  = -1/2+x,1/2-y,1/2+z
   [  2555. ]  = 1/2-x,1/2+y,1/2-z
   [  4565. ]  = 1/2+x,3/2-y,1/2+z
```

Compound 3

Nr	Typ	Res	Donor	---	H	....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	C(13)	--H(13)	..O(9)		[1655.03]	0.95	2.33	3.215(15)	155
2		1	C(20)	--H(20)	..O(8)		[2555.02]	0.95	2.43	3.313(19)	155
3	Intra	1	C(22)	--H(22)	..O(3)		[4455.01]	0.95	2.59	3.074(7)	112

4	Intra 2	C(27) --H(27B) ..O(8)	[	]	0.98	1.85	2.41(5)	113
5	Intra 3	C(30) --H(30C) ..O(9)	[	]	0.98	2.19	2.64(2)	106

:: No Classic Hydrogen Bonds Found

Translation of ARU-code to Equivalent Position Code
==========
[4455.] = -1/2+x,1/2-y,1/2+z
[1655.] = 1+x,y,z
[2555.] = 1/2-x,1/2+y,1/2-z

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification:
G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348

also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
Springer-Verlag, Berlin, 1991, pp 20.

2-Centre (linear) D-H...X most prob. angle 160 deg
3-Centre (bifurcated) SUM of 3 angl. about H = 360 deg
4-Centre (trifurcated)