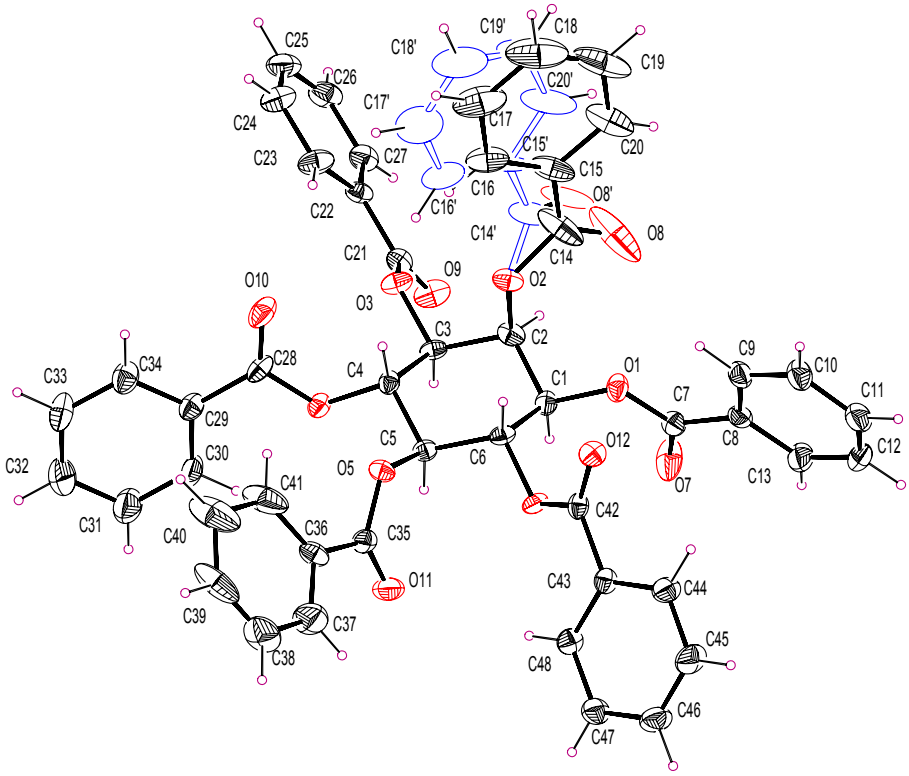
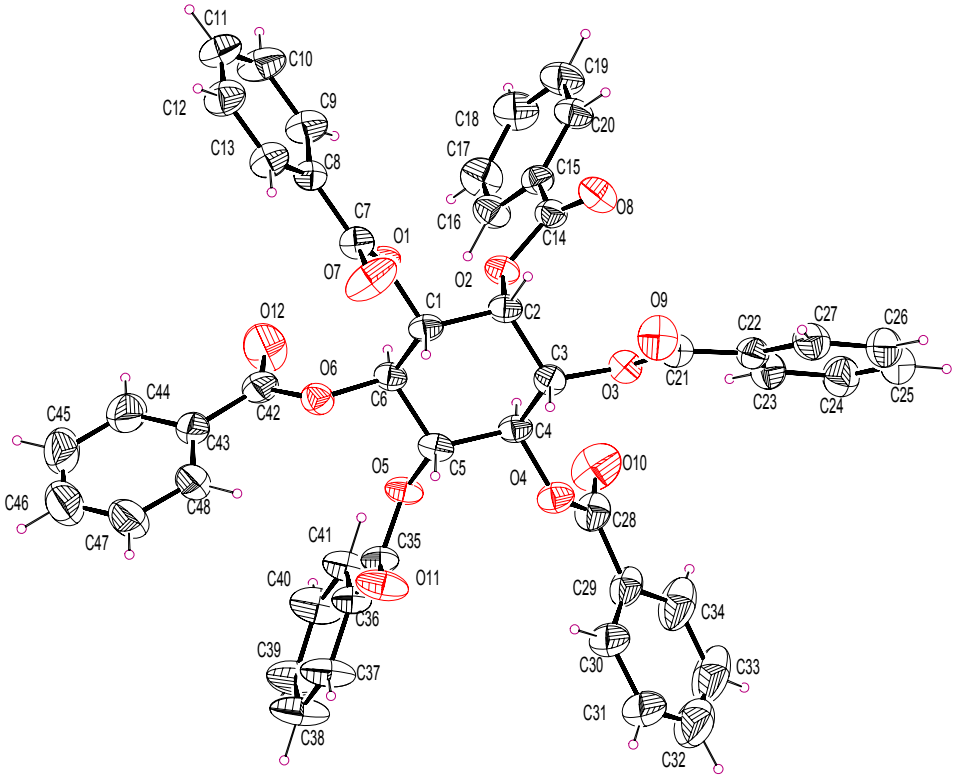
ORTEP View With the Atom Numbering

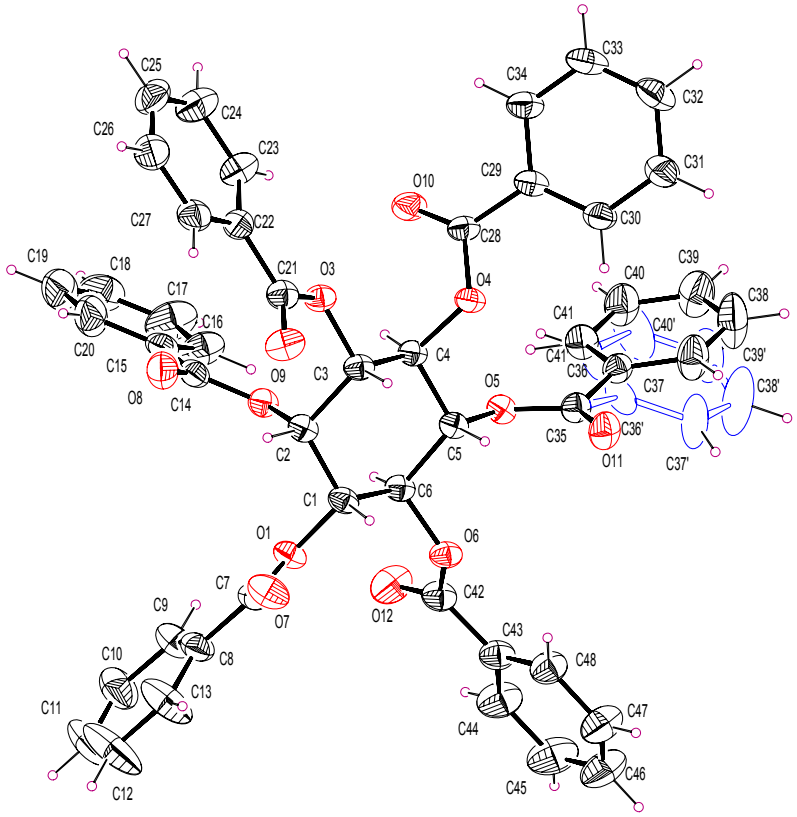
Form I



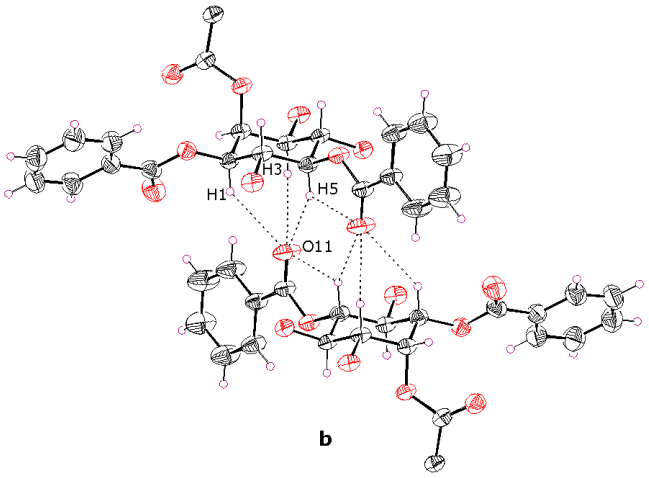
Form II


C11
C10
C12
C9
C13
C8
C7
O1
O7
C19
C18
C20
C17
C15
O8
C16
C14
O2
C1
C2
O9
C22
C27
C26
O12
C3
O6
C6
O3
C21
C23
C24
C25
C44
C45
C42
C4
C43
O5
C5
O4
O10
C46
C48
C28
C47
C41
C35
C40
O11
C29
C34
C36
C39
C37
C30
C33
C31
C38
C32

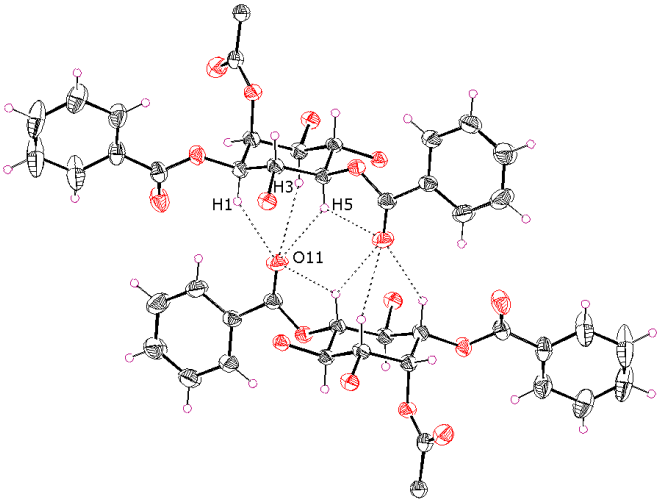
Form III


C33
C34
C32
C25
C24
C31
C26
C23
O10
C29
C27
C22
C28
C30
C19
C18
C21
O3
O4
C40
C39
C17
C38
C41
C40'
C16
C20
C15
O9
C3
C4
C41'
C39'
C36
C37
C38'
O8
C14
O5
C2
C5
C35
C36'
O11
C37'
C1
C6
O1
O6
C7
C42
O12
C9
O7
C43
C10
C8
C48
C13
C11
C44
C47
C12
C45
C46

Similarity in Centrosymmetrically Trifurcated Bridged Pair-Form II and Form III



Form II



Form III

Only Form II is given in the manuscript because of the similarity of this Form with III. The geometry of interactions within this pair is given below:

C-H…O Interactions in Form II (again recorded for easy comparison with III)

D-H...A	d(D-H) Å	d(H...A) Å	d(D...A) Å	<(D-H…A)°
C(1)-H(1)...O(11)#1	0.98	2.48	3.340(3)	146.9
C(3)-H(3)...O(11)#1	0.98	2.70	3.514(3)	140.2
C(5)-H(5)...O(11)#1	0.98	2.48	3.335(3)	145.4

C-H…O Interactions in Form III

D-H...A	d(D-H) Å	d(H...A) Å	d(D...A) Å	<(D-H…A) °
C(1)-H(1)...O(11)#2	0.98	2.40	3.249(3)	144.4
C(3)-H(3)...O(11)#2	0.98	2.51	3.335(3)	141.7
C(5)-H(5)...O(11)#2	0.98	2.67	3.444(3)	136.3

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

Intermolecular Weak Interactions in Forms I, II and III:

Apart from the C-H…O interactions highlighted in our manuscript, which link the nearest pairs, there are other interactions as well in all the three forms. They are given here for ready reference.

C-H…π Interaction in Forms I, II and III

Form I

X--H(I) Cg(J)	H..Cg (Å)	H-Perp (Å)	X-H..Cg (°)	X..Cg (Å)
C(33) -H(33)… $Cg(7)^{3}$	3.2535	3.176	141.04	4.0193
C(38) -H(38)… $Cg(2)^{1}$	3.1047	3.028	161.97	3.9994
C(47) -H(47)… $Cg(4)^{2}$	2.9101	2.853	148.82	3.7369
C(19') -H(19')…$Cg(6)^{10}$	3.1049	2.958	145.57	3.9075

Form II

C(10) -H(10)…$Cg(4)^{6}$	2.8496	2.845	140.57	3.6165
C(45) -H(45)…$Cg(5)^{3}$	2.9975	2.772	140.90	3.7652
C(26) -H(26)…$Cg(2^{5}$	2.8431	2.785	146.14	3.6523
C(33) -H(33)…$Cg(3)^{8}$	2.9484	2.829	138.04	3.6926

Form III

C(24) -H(24)…Cg(5)[9]	3.1517	3.082	141.77	3.9247
C(33) -H(33)…Cg(3)[9]	3.1693	3.120	141.04	3.9361
C(50) -H(50A)…Cg(4)[4]	3.3300	3.311	130.59	4.0291

π…π Interactions in Form I, II and III

There are no significant π…π interactions in Forms I and II; Form III has a single π…π interaction as given below

Cg(I)	Cg(J)	Cg-Cg (Å)	Alpha (°)	CgI_perp (Å)	CgJ_perp (Å)
Cg(2)	Cg(2)[7]	3.877	0.00	3.835	3.835

Alpha – Dihedral angle between planes I and J in Degree.

Cg 2 = C8-C13, Cg 3 = C15-C20, Cg 4 = C22-C27, Cg 5 = C29-C34, Cg 6 = C36-C41, Cg 7 = C43-C48, Cg 3'= C15'-C20'

[1] -1+X,-1+Y,Z; [2] -1+X,Y,Z; [3] X,-1+Y,Z ; [4] –1+X, -1+Y,-1+Z; [5] X,1+Y,Z; [6] -X,1-Y,1- Z; [7] 2-X,3-Y,2-Z; [8] -X,2-Y,-Z; [9] 3-X,3-Y,1-Z ; [10] 1+Y,1-X+Y,-1/6+Z

Other C-H…O Interactions in Forms I, II and III

Form I [Å and deg (°)]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9)...O(7)#1	0.93	2.87	3.435(5)	120.1
C(10)-H(10)...O(7)#1	0.93	2.88	3.436(6)	119.5
C(12)-H(12)...O(10)#4	0.93	2.48	3.334(5)	152.1
C(25)-H(25)...O(11)#6	0.93	2.52	3.322(5)	144.3
C(27)-H(27)...O(10)#3	0.93	2.42	3.227(5)	145.0
C(39)-H(39)...O(7)#5	0.93	2.63	3.538(6)	164.8
C(44)-H(44)...O(11)#1	0.93	2.69	3.376(5)	131.7
C(46)-H(46)...O(8')#2	0.93	2.58	3.486(11)	165.2

Symmetry Code: #1 y,-x+y+1,z-1/6 #2 x-1,y,z #3 x-y+1,x,z+1/6 #4 x,y+1,z #5 y-1,-x+y,z-1/6 #6 x+1,y,z

Form II [Å and deg (°)]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(18)-H(18)...O(9)#3	0.93	2.79	3.673(4)	158.1
C(19)-H(19)...O(7)#5	0.93	2.91	3.658(4)	137.9
C(24)-H(24)...O(10)#4	0.93	2.77	3.613(4)	151.5
C(41)-H(41)...O(12)#2	0.93	2.52	3.228(4)	133.4
C(48)-H(48)...O(4)#1	0.93	2.91	3.650(4)	137.3

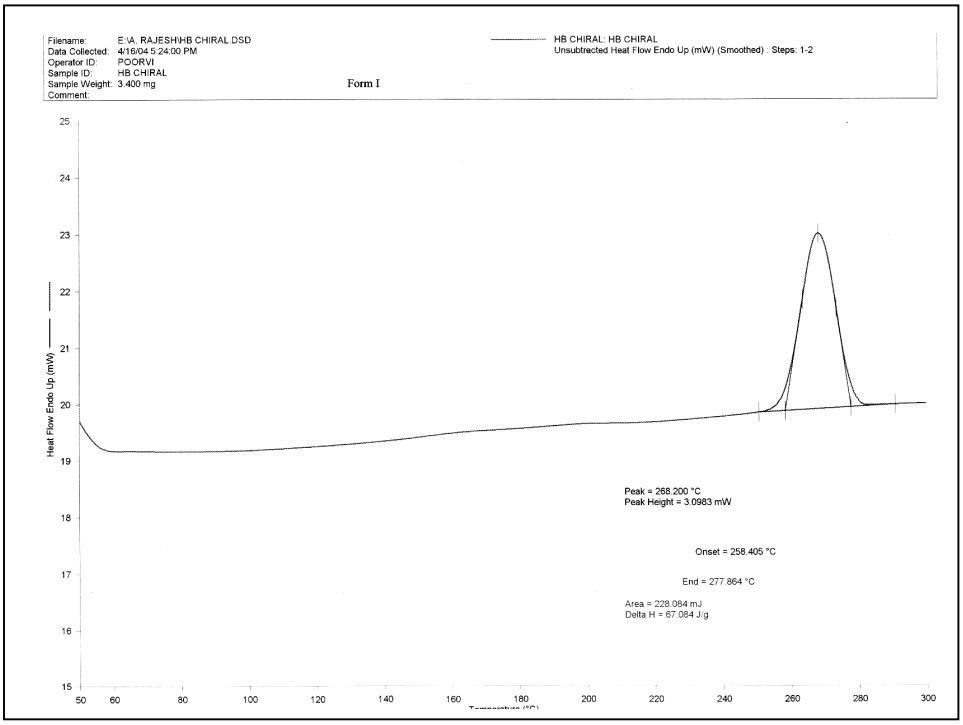
Symmetry Code: #1 -x+1,-y+1,-z #2 -x,-y+1,-z #3 x-1,y,z #4 -x,-y+2,-z #5 -x,-y+1,-z+1

Form III [Å and deg (°)]

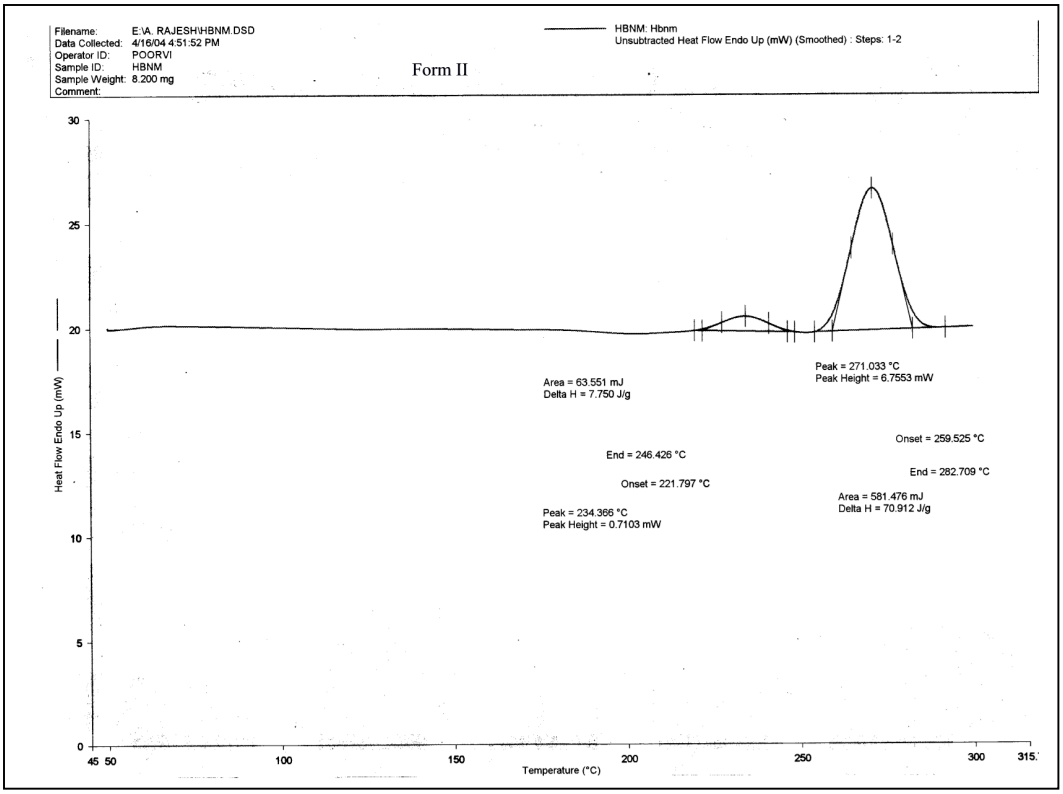
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11)...O(8)#3	0.93	2.52	3.365(4)	150.5
C(17)-H(17)...O(12)#4	0.93	2.50	3.230(6)	135.2
C(34)-H(34)...O(10)#5	0.93	2.53	3.400(4)	155.6
C(37)-H(37)...O(7)#2	0.93	2.62	3.404(5)	142.6
C(48)-H(48)...O(4)#2	0.93	2.71	3.516(3)	145.6
C(49)-H(49B)...O(10)#1	0.97	2.63	3.375(5)	133.4
C(49)-H(49A)...O(12)#4	0.97	2.40	3.232(4)	143.2
C(50)-H(50B)...O(9)#2	0.97	2.59	3.104(6)	113.1
C(27)-H(27)...O(8)#6	0.93	2.82	3.489(4)	129.7

Symmetry Code: #1 x-1,y-1,z #2 –x+2,-y+2,-z+1 #3 –x+2,-y+3,-z+2 #4 –x+2,-y+3,-z+1 #5 -x+3,-y+3,-z+1 #6 -x+3,-y+3,-z+2

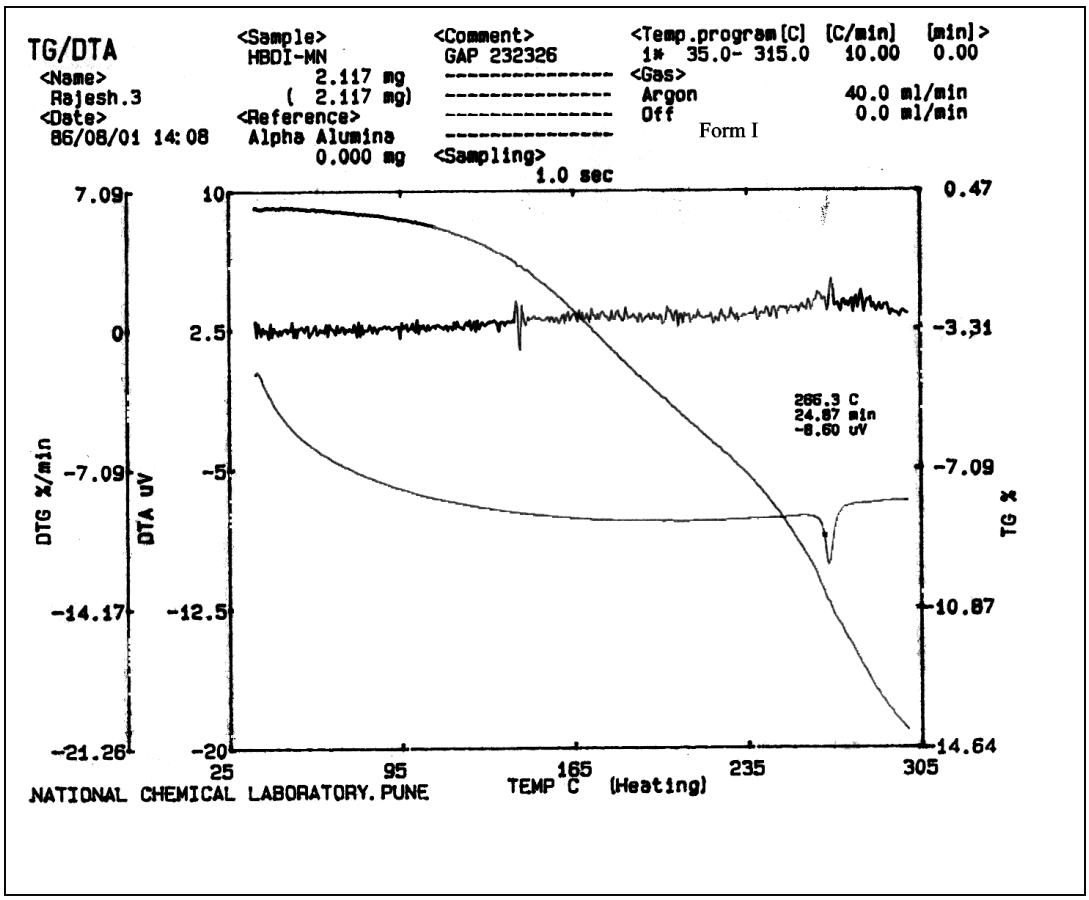
1) DSC of Form I



2) DSC of Form II



3) TG / DTA of Form I



4) TG / DTA of Form II