Solvent Induced Crystallization of 1,2,3,4(6),5-Penta-*O*-Acetyl-6(4)-*O*-[(1S)-10-Camphor Sulfonyl]-*myo*-Inositol Diastereomers Associated *via* Weak Trifurcated C–H···O Interactions

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Supplementary Information

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Figure SF1: DTA/TGA plots of (a) **1·1DCM**; (b) **1·2AN**; (c) **1·2NM**; (d) **1·2AC**; (e) **1·2CF**; (f) **1·2DCE**.

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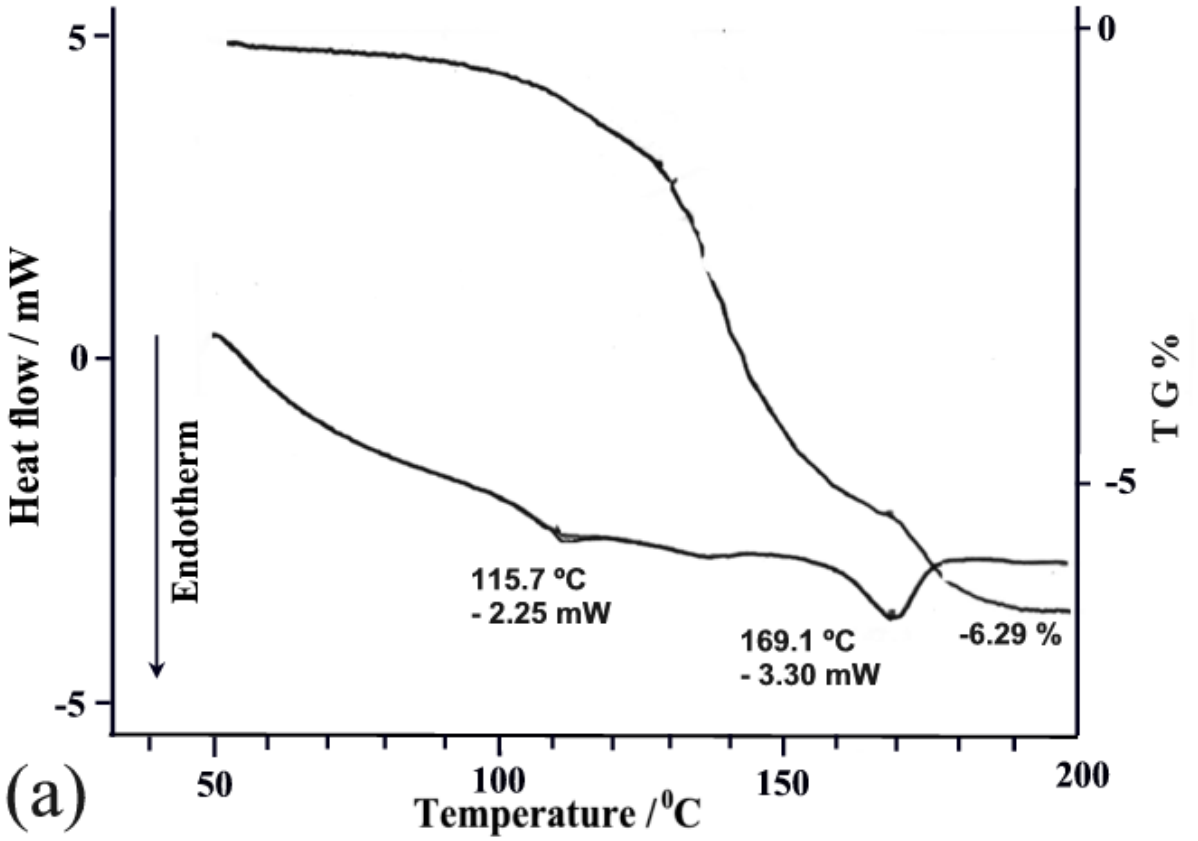
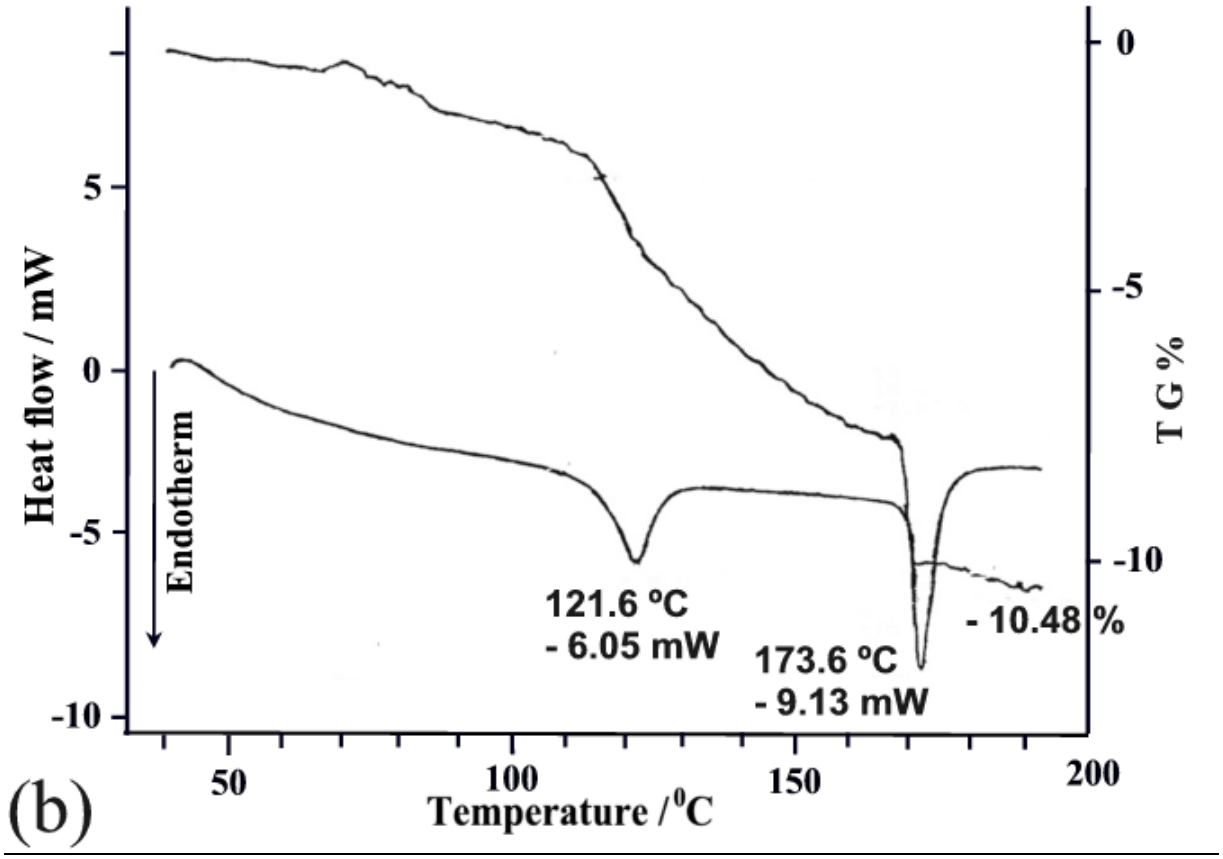
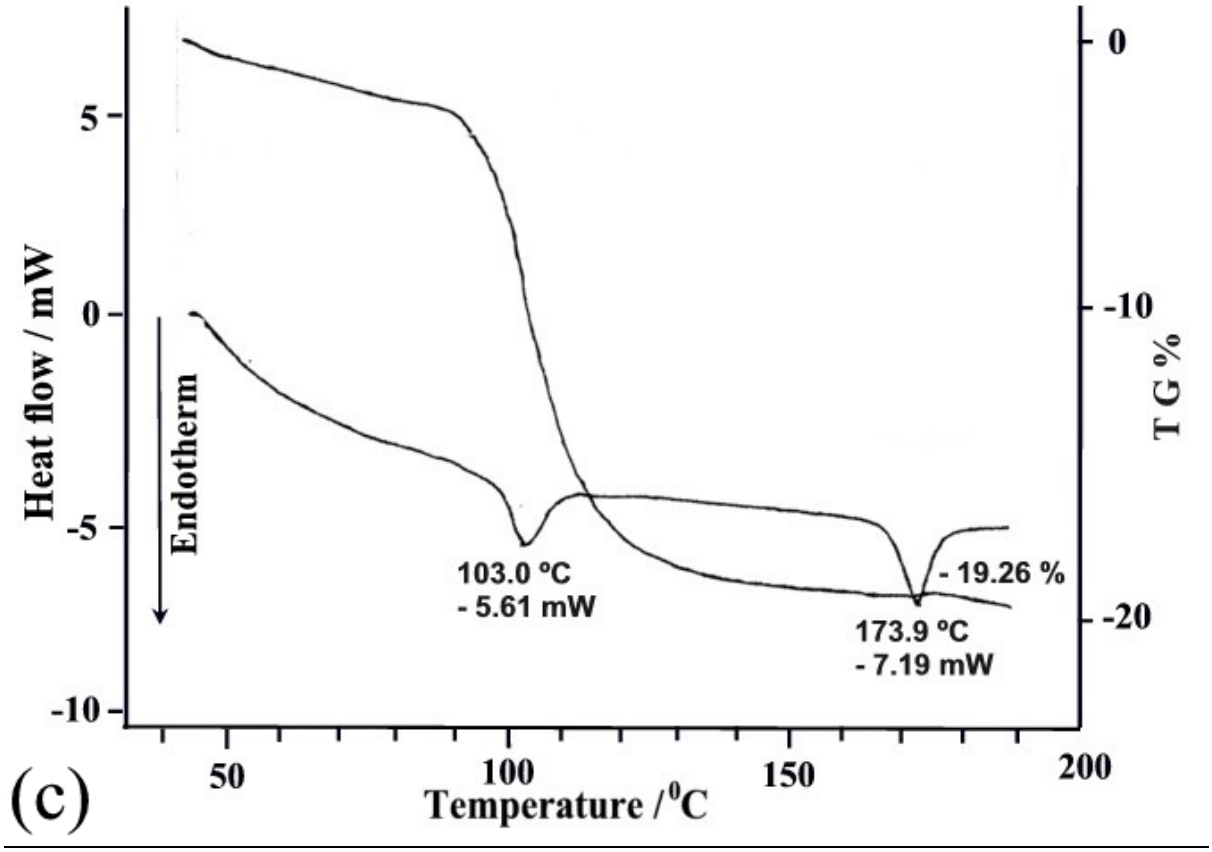
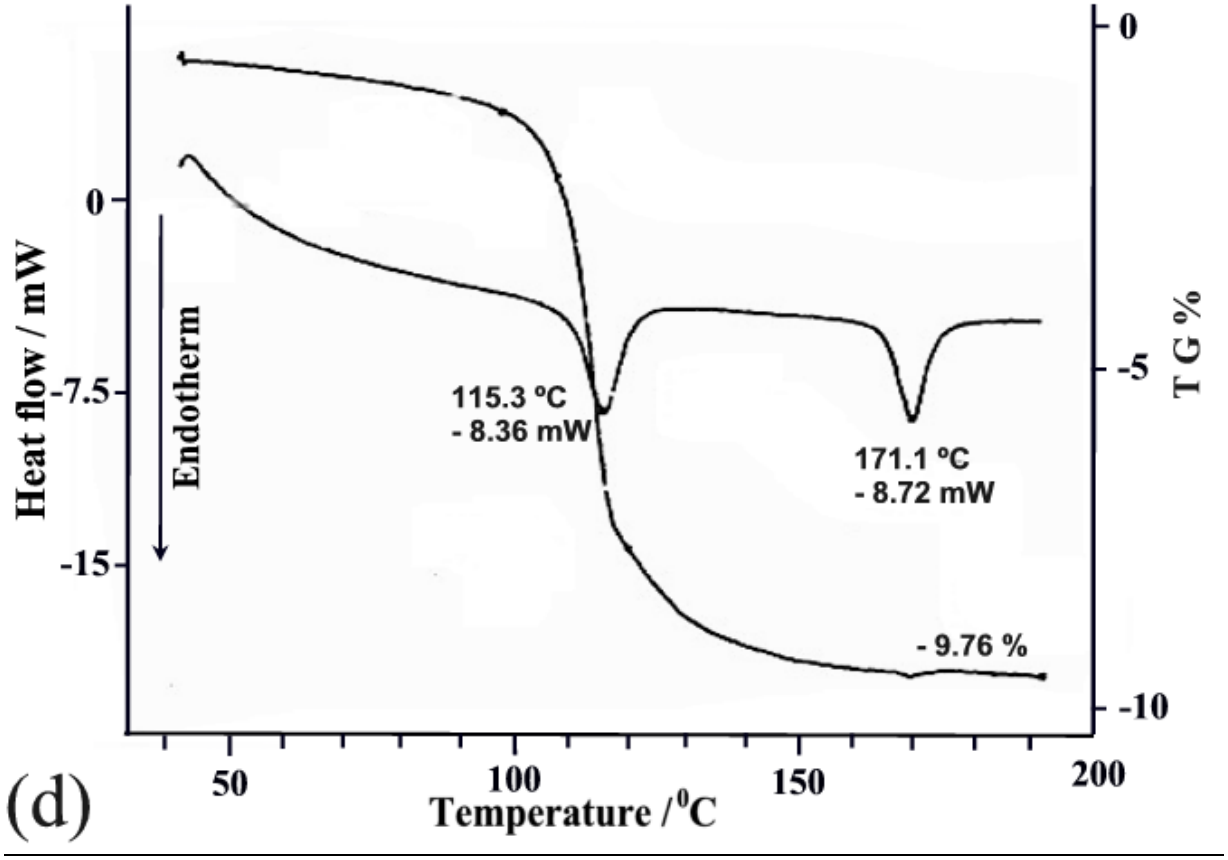
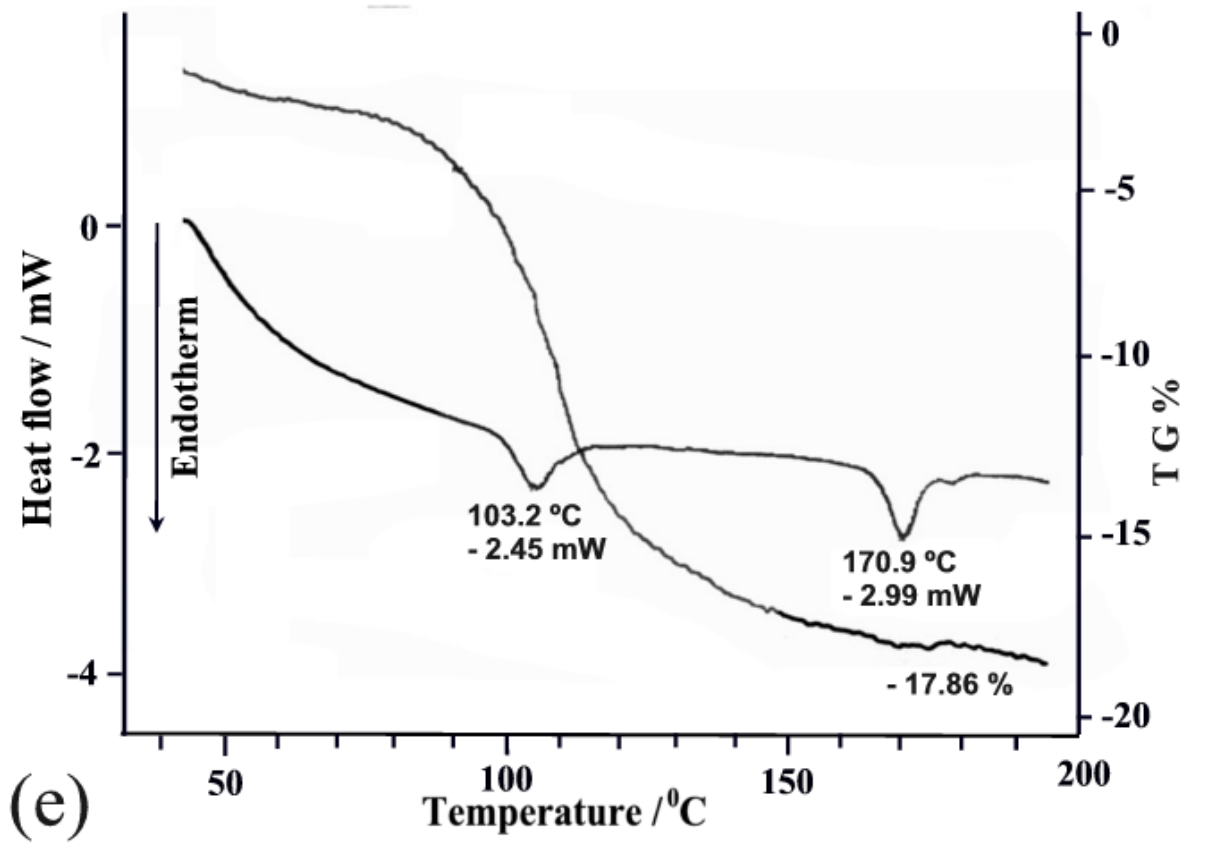










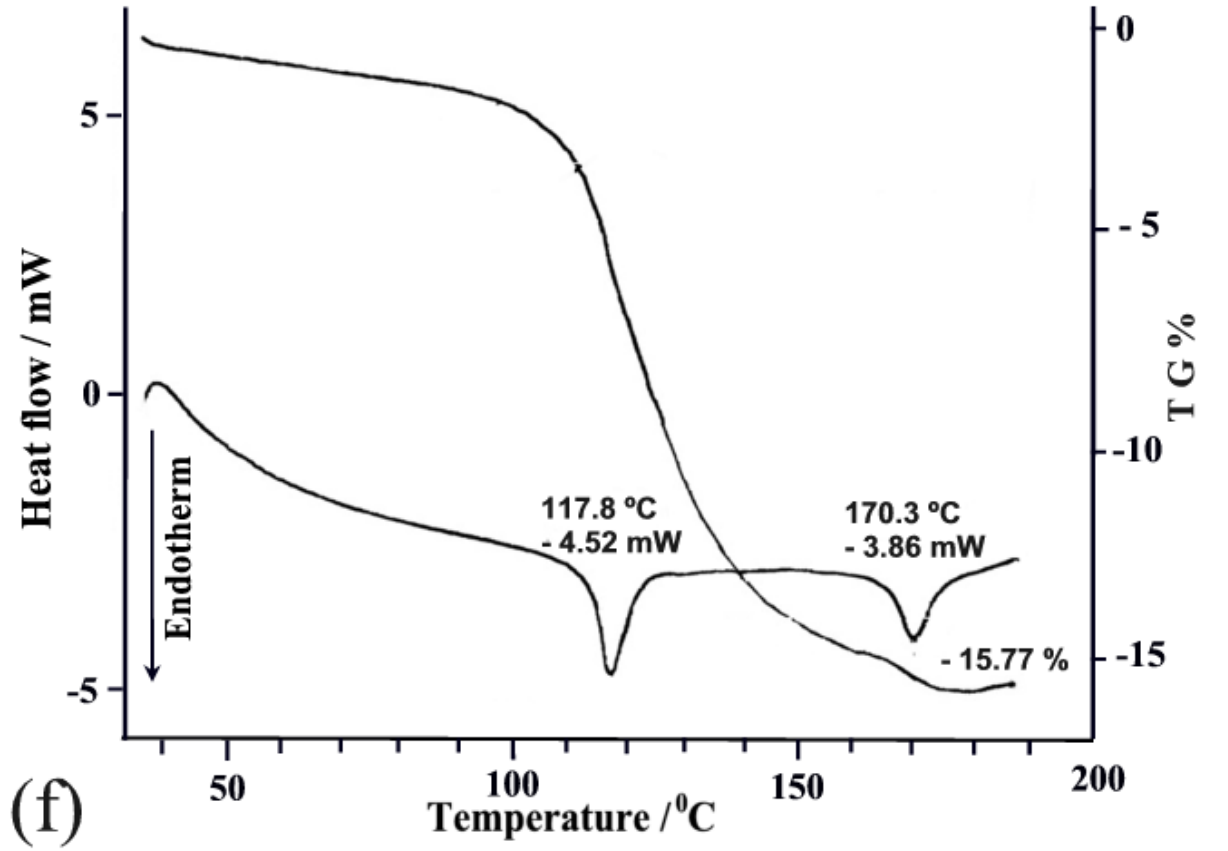
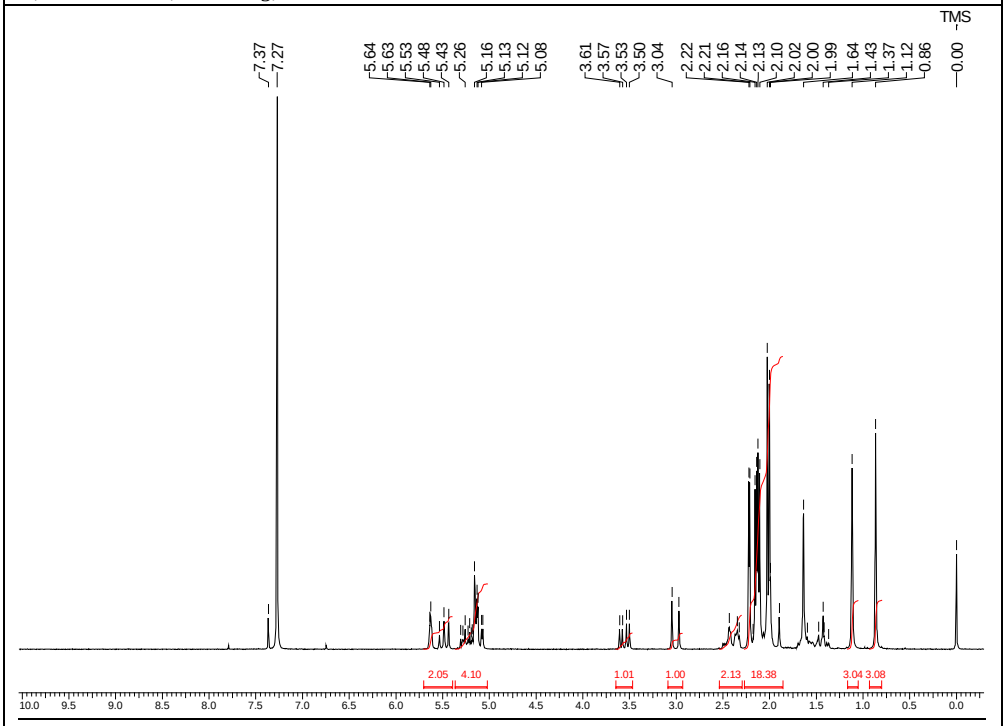
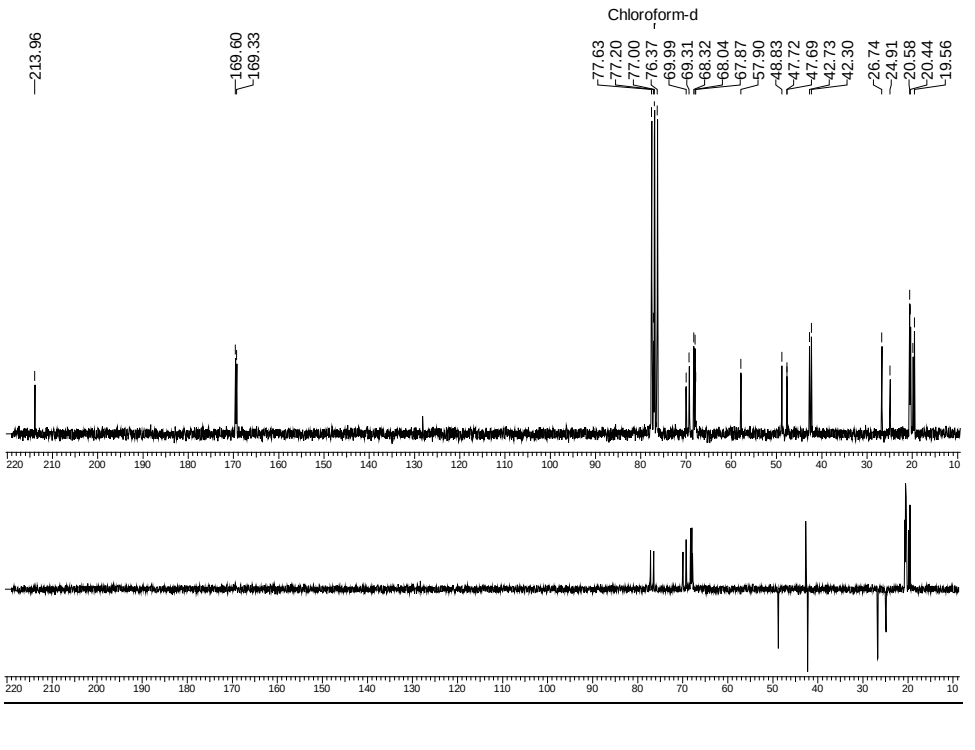


Figure SF2: 1H NMR spectra of **1** and its solvates ($CDCl_3$, 200 MHz).

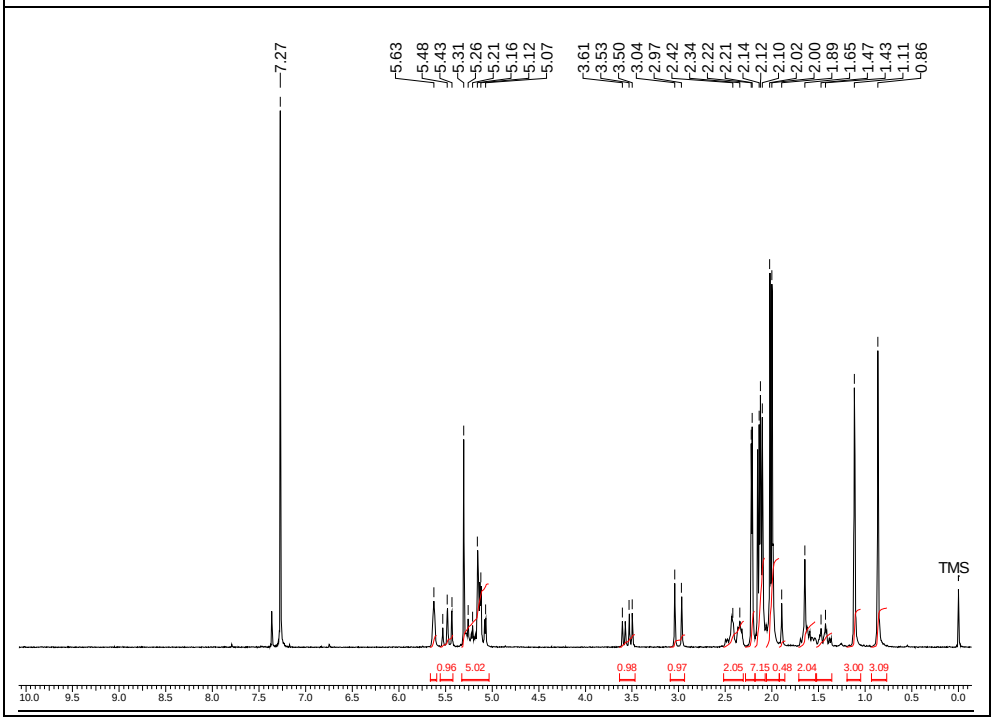
1, 1H NMR, $CDCl_3$, 200 MHz



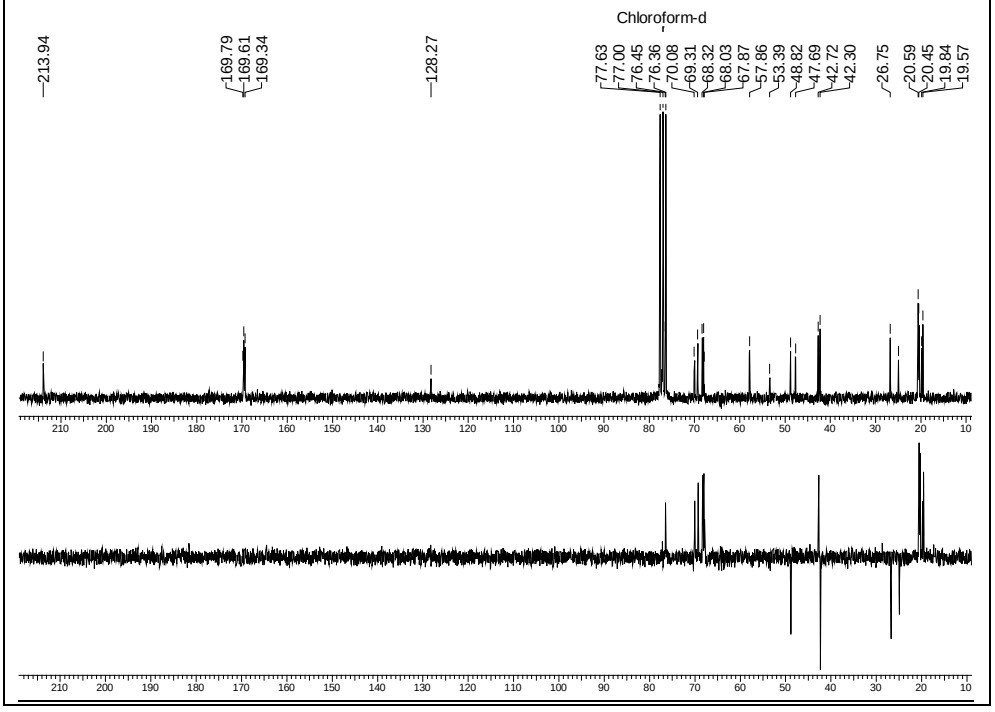
1, ^{13}C NMR and Dept, 50 MHz



1.1 DCM, 1H NMR, $CDCl_3$, 200 MHz



1.1 DCM, ^{13}C NMR, and Dept, 50 MHz



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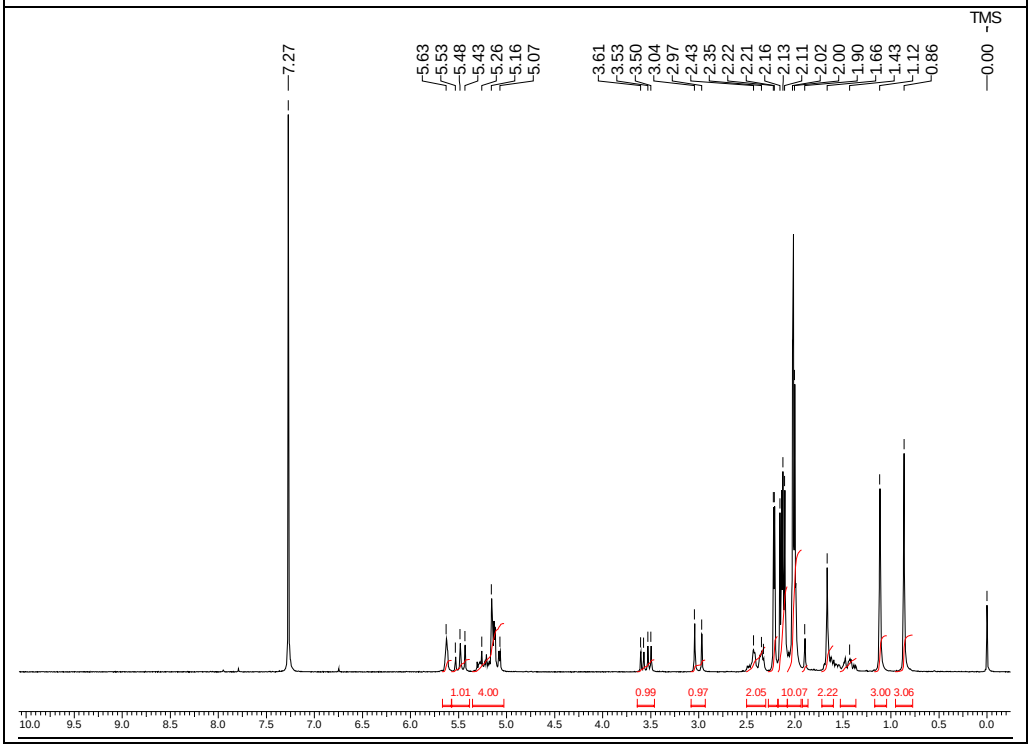
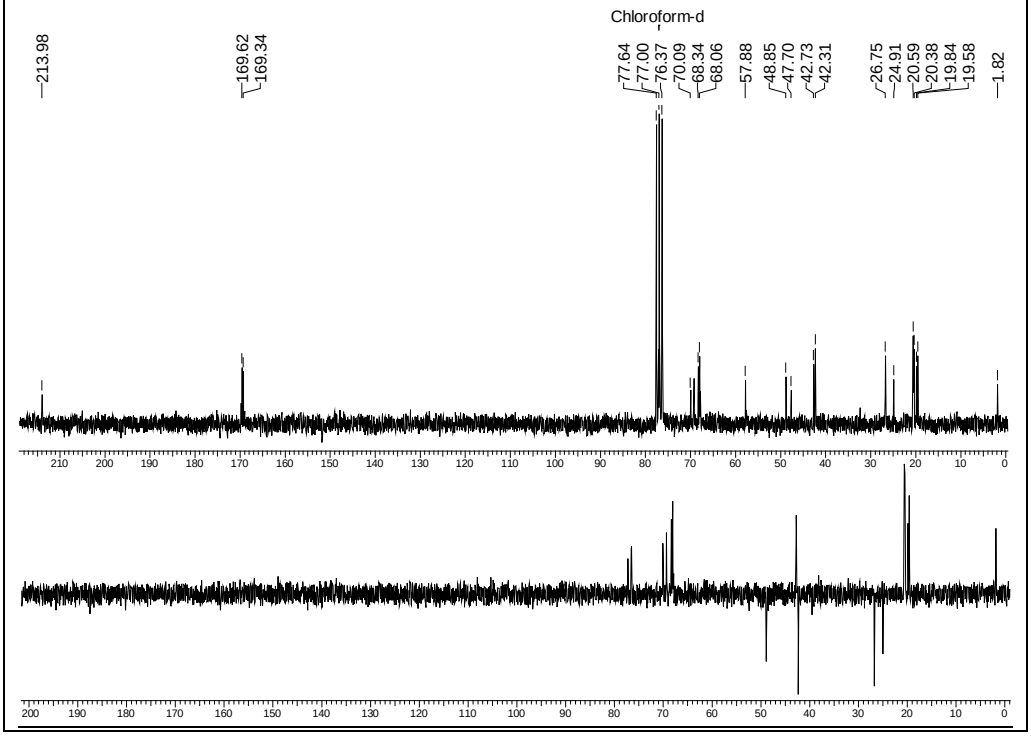
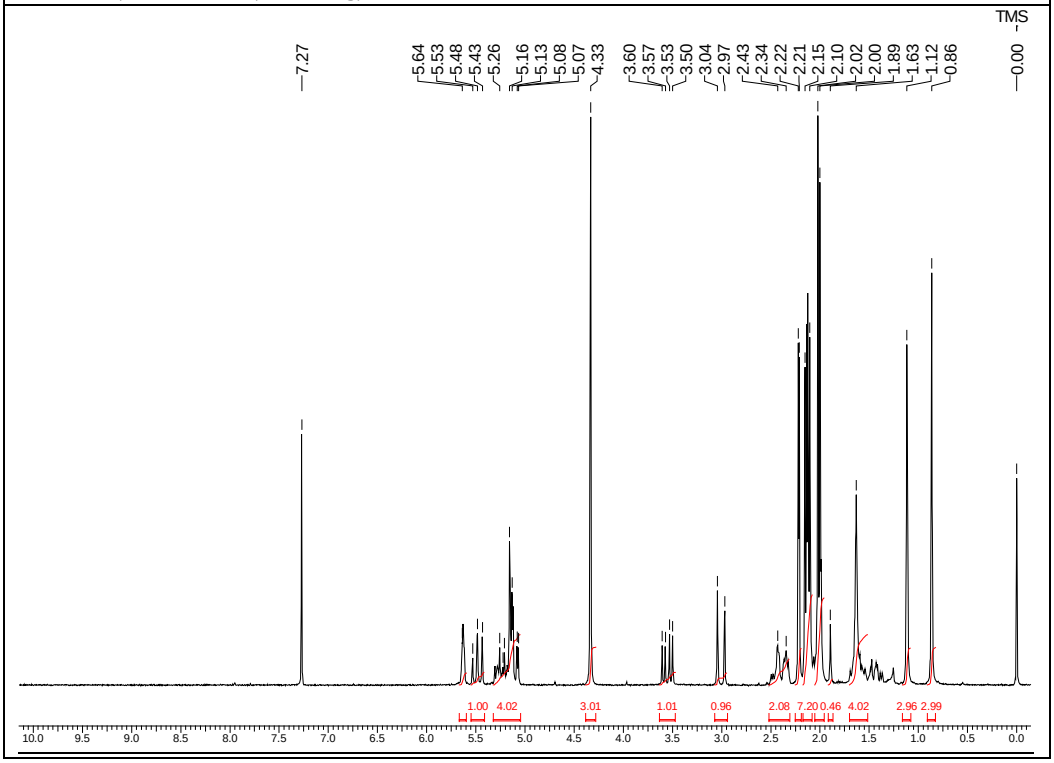


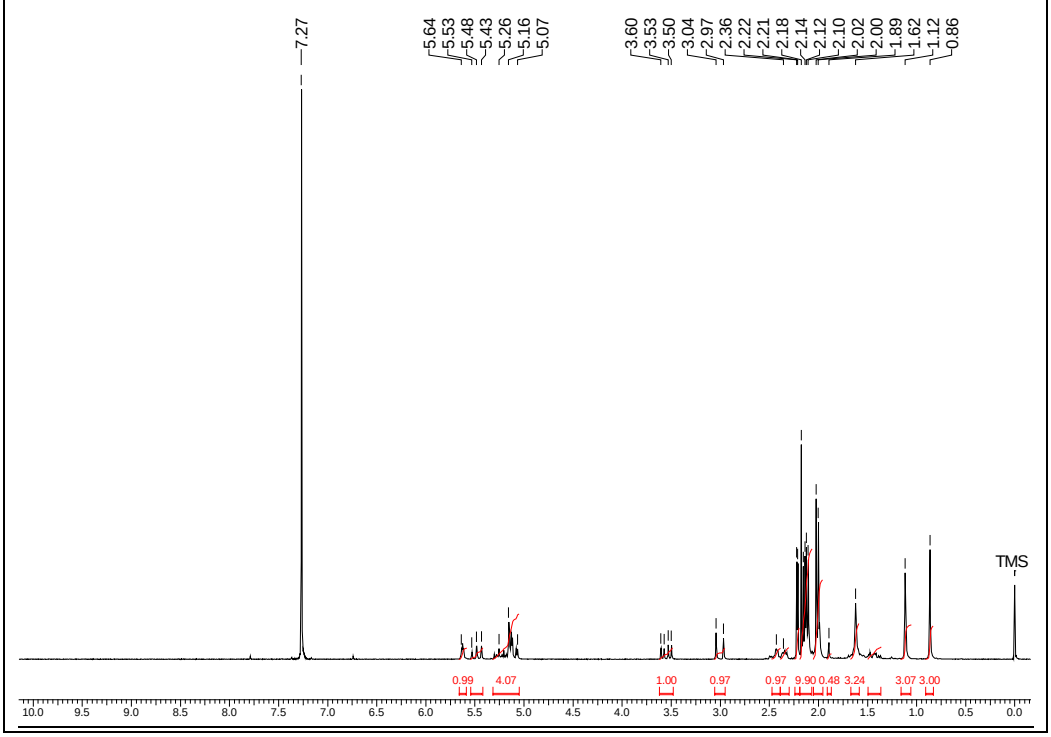
1.2 AN, ^{13}C NMR and Dept, $CDCl_3$, 50 MHz



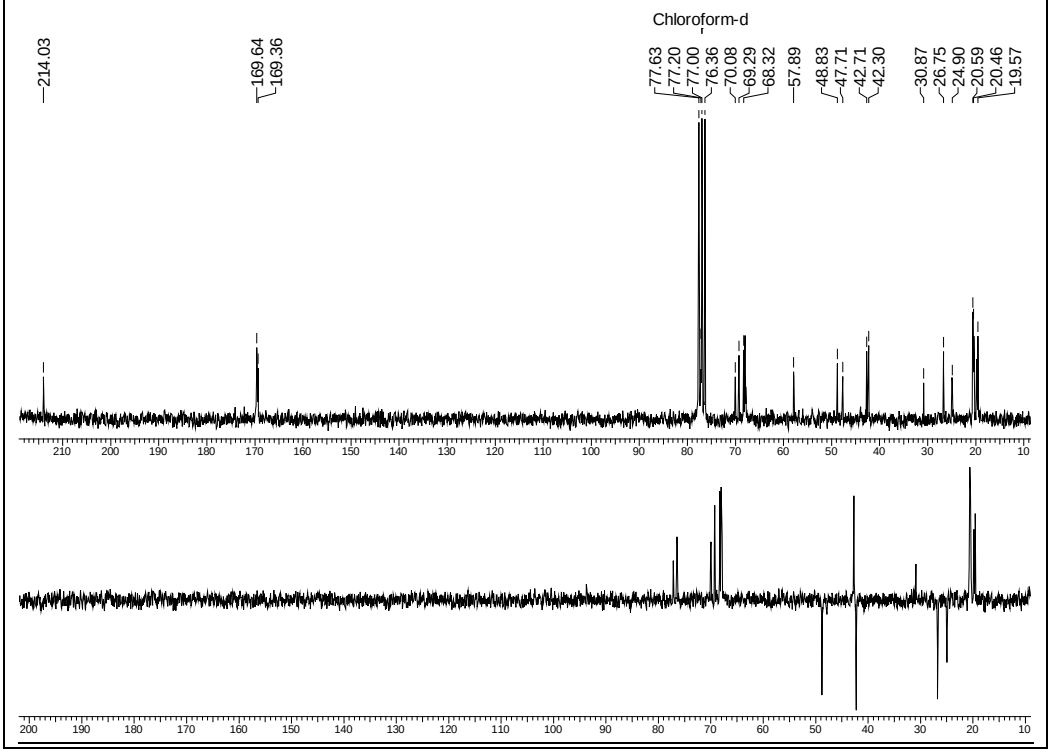
1.2 NM, 1H NMR, $CDCl_3$, 200 MHz



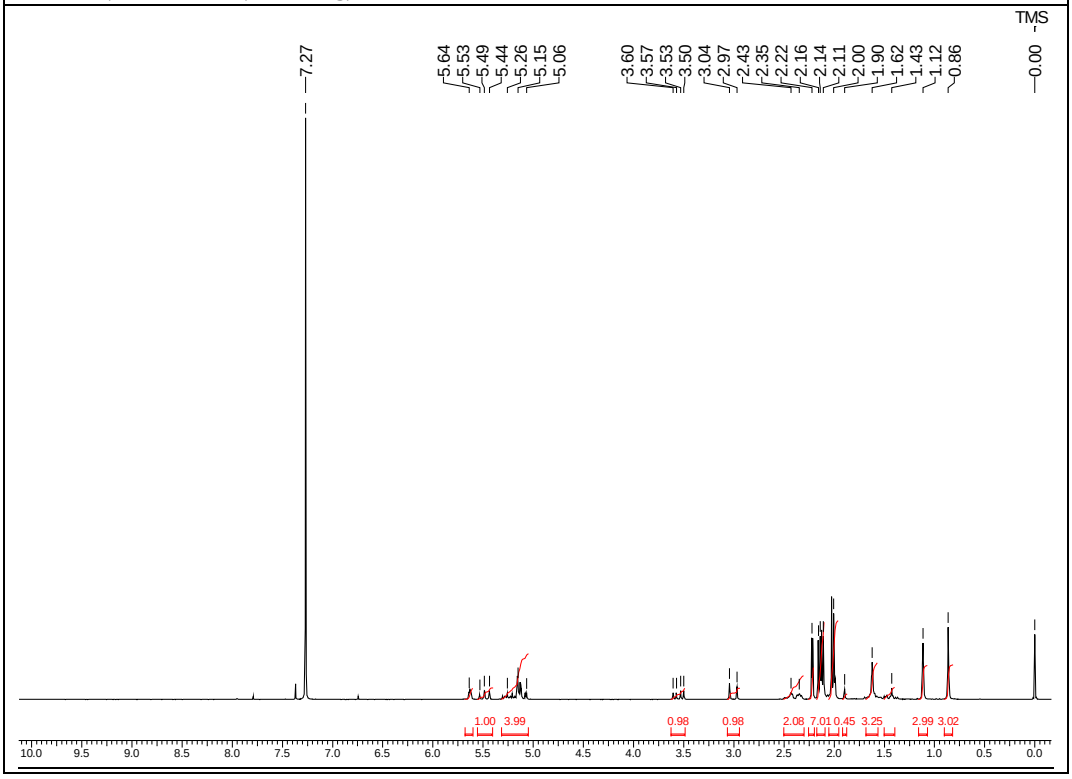
1.2 AC, 1H NMR, $CDCl_3$, 200 MHz



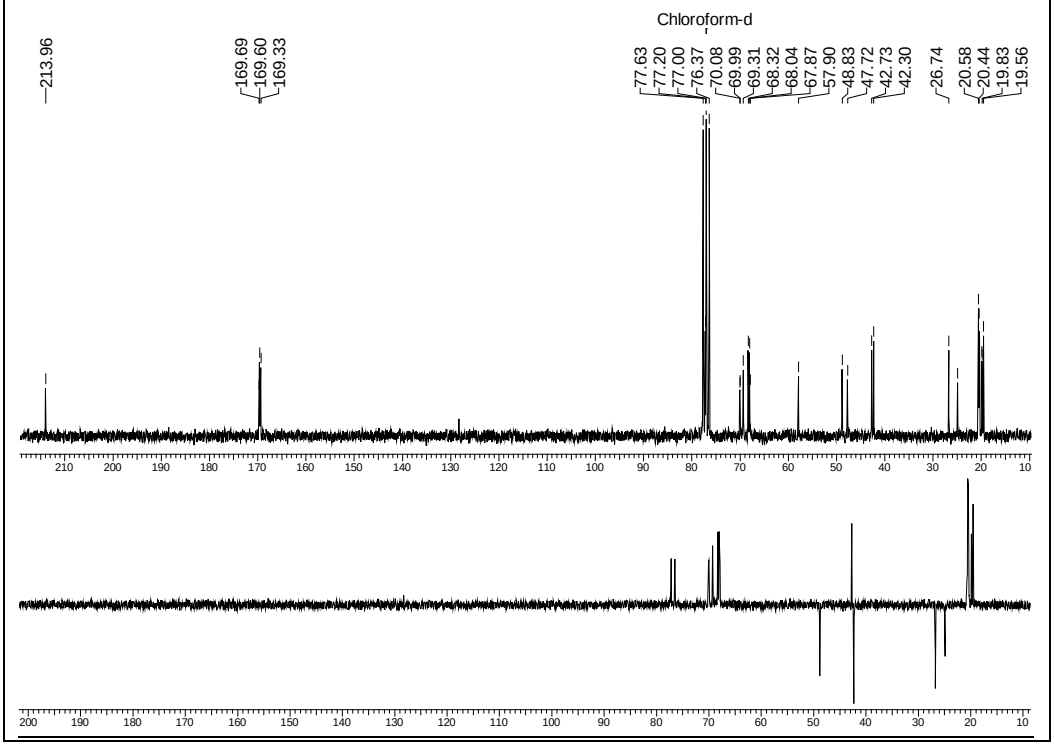
1.2 AC, ^{13}C NMR and Dept, $CDCl_3$, 50 MHz



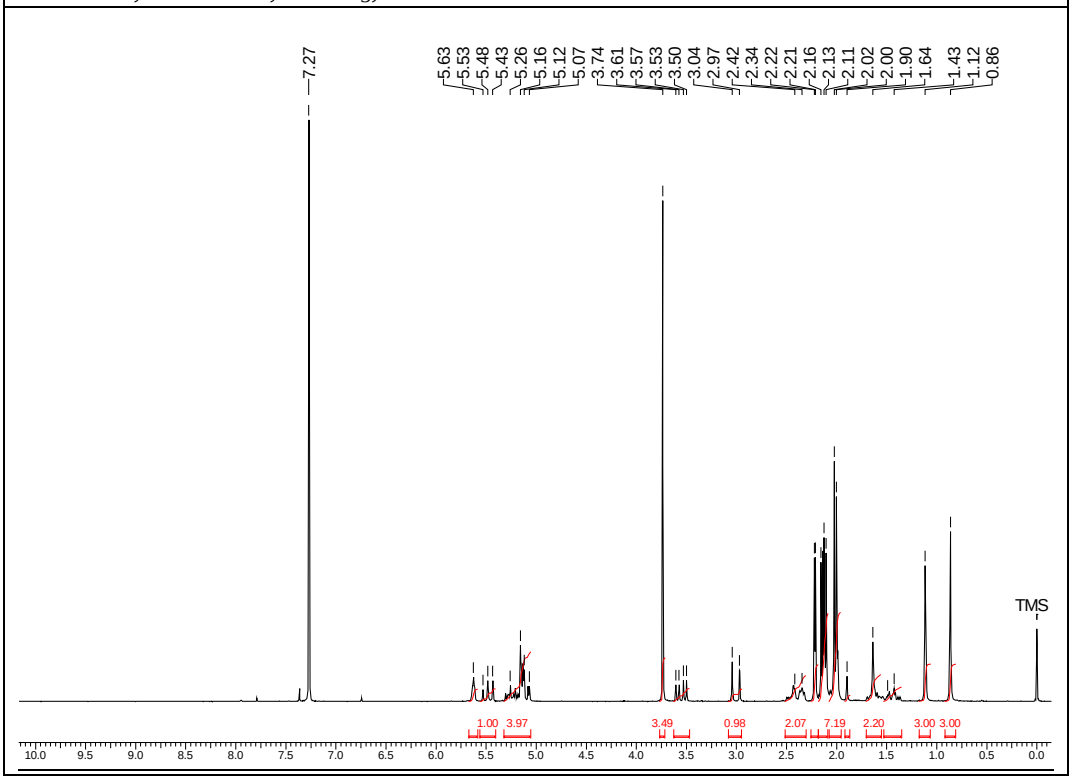
1.2 CF, 1H NMR, $CDCl_3$, 200 MHz



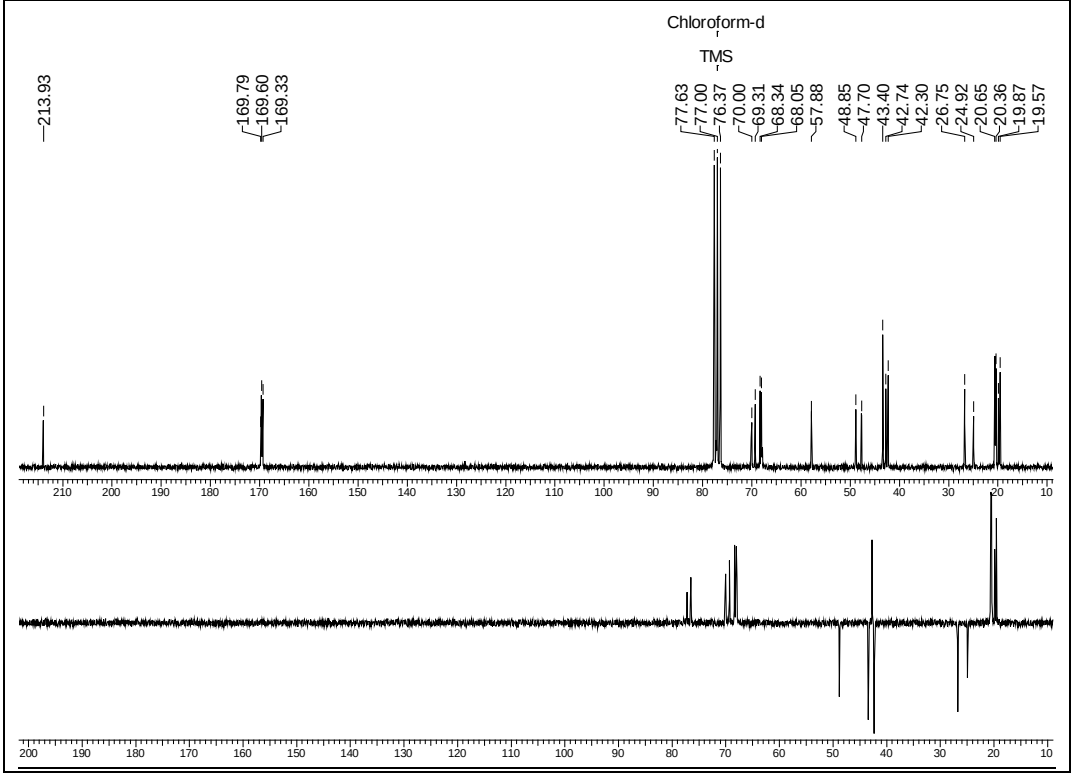
1.2 CF, ^{13}C NMR and Dept, $CDCl_3$, 50 MHz



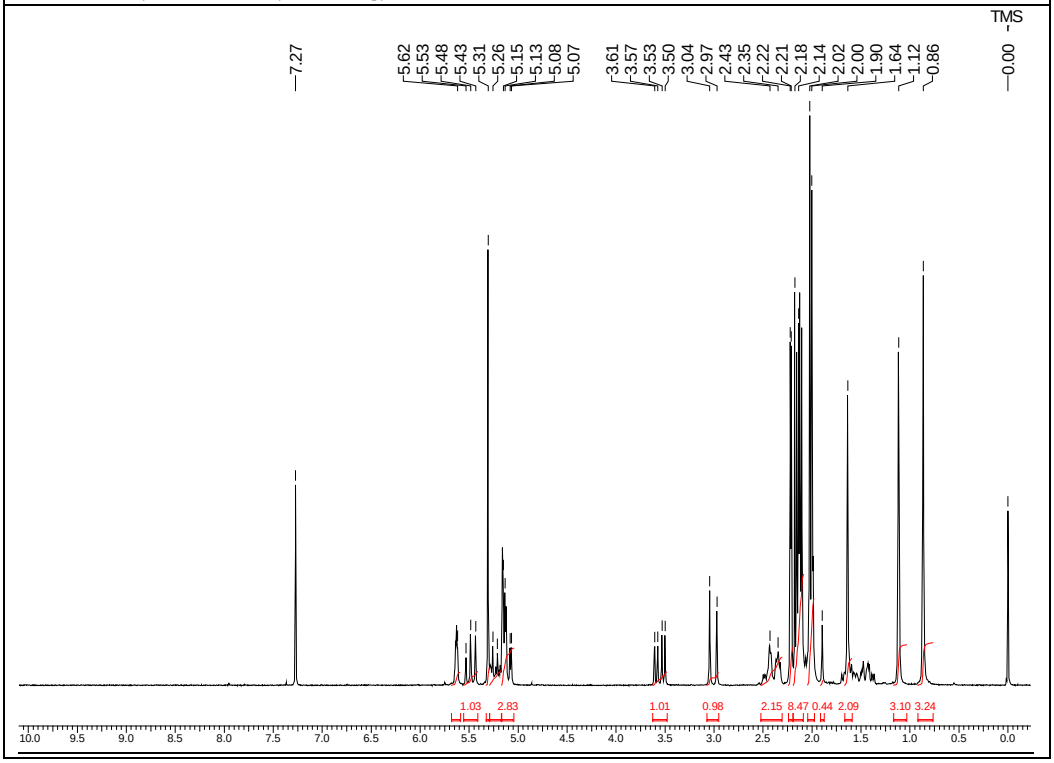
1.2 DCE, 1H NMR, $CDCl_3$, 200 MHz



1.2 DCE, ^{13}C NMR and Dept, $CDCl_3$, 50 MHz



1.2 DCM, 1H NMR, $CDCl_3$, 200 MHz



Crystallographic details of least-square refinement

Full-matrix least-squares refinements of Type I and III crystals were carried out by applying geometrical and anisotropic displacement constraints (DFIX, DANG, SIMU and DELU) in *SHELXL97* to retain their molecular geometries close to their ideal values. These constraints were applied particularly to the guest molecules in **1·1DCM** and **1·2CF**, and camphorsulfonate group of the host in **1·2DCE** and **1·2DCM** crystals. Most of the included guest solvents in Type II and III showed statistical disorder in their crystal lattice. The oxygen atoms O17 and O18 of the nitromethane guest in site *A* [*please refer figure* 4] disordered over two positions (O17' and O18') having 0.5 occupancy each, whereas in site *B* [*please refer figure* 4], all the atoms are disordered over two positions with equal occupancies in **1·2NM**. In **1·2AC**, the oxygen atoms (O15 and O16) of both the acetone molecules indicated two positions (O15' and O16') with occupancies 0.25 and 0.375 respectively. The guest in site *A* of **1·2CF** crystals also showed two different locations for chloroform molecule with occupancies 0.5 and 0.25 respectively. In **1·2DCE** crystals, two positions of chlorine atoms were assigned at site *B* with occupancies 0.875 (for Cl3 and Cl4) and 0.125 (for Cl3' and Cl4') respectively. Traces of water molecules (O15 and O16) in **1·2AN** were picked up in the difference Fourier, which were assigned occupancies of 0.35 and 0.15 respectively. A single water molecule (O1*W*) having a lower occupancy (0.25) was also located along with nitromethane in the difference Fourier in **1·2NM**.

Figure SF3: Molecular overlap figure of diastereomers **1** (*a*) diastereomer with unprimed labeling and (*b*) diastereomer with primed labeling [Black: **1·1DCM**, Blue: **1·2AN**, Green: **1·2NM**, Red: **1·2AC**, Purple: **1·2CF**, Orange: **1·2DCE**, Violet: **1·2DCM**].

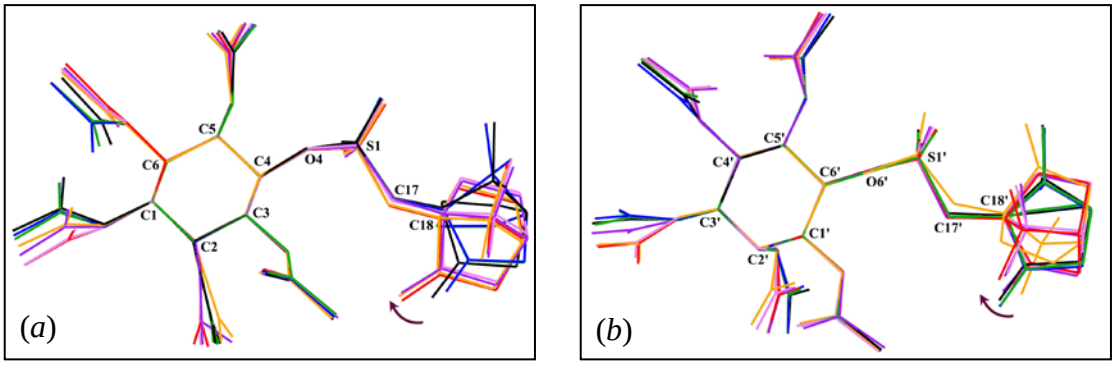


Figure SF4: Molecular layer figures of diastereomers **1** in the third dimension (*a*) Type I [**1·1DCM**], (*b*) Type II [**1·2AN**] and (*c*) Type III [**1·2DCM**] crystals (dimeric units are shown in red and blue).

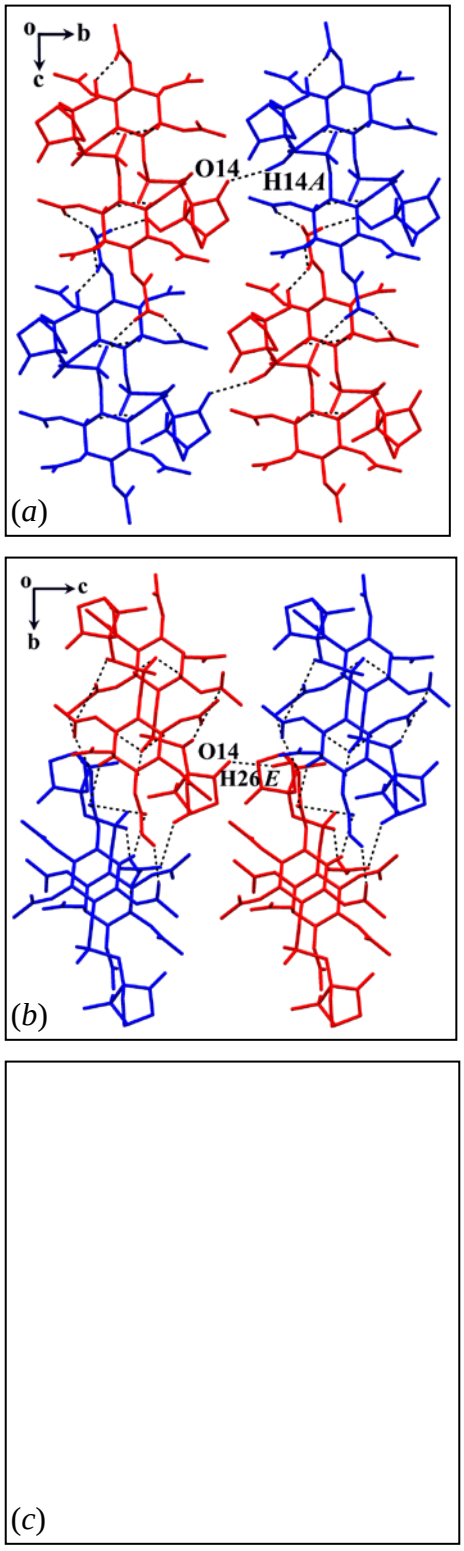


Table ST1: Geometrical parameters for trifurcated C–H···O interactions shown in figure 3.

Crystals	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
1·1DCM	C1–H1···O13'	0.98	2.80	3.601(8)	139
	C3–H3···O13'	0.98	2.54	3.382(10)	145
	C5–H5···O13'	0.98	2.54	3.385(9)	145
	C1'–H1'···O13	0.98	2.49	3.325(10)	143
	C3'–H3'···O13	0.98	2.73	3.539(8)	140
	C5'–H5'···O13	0.98	2.48	3.322(8)	144
1·2AN	C1–H1···O13'	0.98	2.79	3.583(5)	139
	C3–H3···O13'	0.98	2.57	3.434(3)	147
	C5–H5···O13'	0.98	2.62	3.455(4)	143
	C1'–H1'···O13	0.98	2.53	3.381(3)	145
	C3'–H3'···O13	0.98	2.69	3.498(5)	140
	C5'–H5'···O13	0.98	2.59	3.413(4)	142
1·2NM	C1–H1···O13'	0.98	2.79	3.589(12)	140
	C3–H3···O13'	0.98	2.61	3.460(8)	147
	C5–H5···O13'	0.98	2.65	3.484(10)	143
	C1'–H1'···O13	0.98	2.55	3.403(8)	145
	C3'–H3'···O13	0.98	2.65	3.461(11)	141
	C5'–H5'···O13	0.98	2.60	3.423(9)	142
1·2AC	C1–H1···O13'	0.98	2.55	3.405(1)	146
	C3–H3···O13'	0.98	2.59	3.434(1)	144
	C5–H5···O13'	0.98	2.74	3.537(1)	139
	C1'–H1'···O13	0.98	2.50	3.357(1)	146
	C3'–H3'···O13	0.98	2.61	3.415(1)	140
	C5'–H5'···O13	0.98	2.76	3.543(1)	137
1·2CF	C1–H1···O13'	0.98	2.46	3.382(6)	158
	C3–H3···O13'	0.98	2.85	3.654(6)	139
	C5–H5···O13'	0.98	2.85	3.727(5)	137

	C1'–H1'···O13	0.98	2.67	3.487(6)	141
	C3'–H3'···O13	0.98	2.46	3.338(6)	149
	C5'–H5'···O13	0.98	2.86	3.630(5)	136
1·2DCE	C1–H1···O13'	0.98	2.46	3.328(6)	147
	C3–H3···O13'	0.98	2.51	3.362(7)	145
	C5–H5···O13'	0.98	2.82	3.591(7)	136
	C1'–H1'···O13	0.98	2.46	3.402(7)	160
	C3'–H3'···O13	0.98	2.89	3.720(8)	144
	C5'–H5'···O13	0.98	2.66	3.495(7)	143
1·2DCM	C1–H1···O13'	0.98	2.54	3.405(8)	148
	C3–H3···O13'	0.98	2.58	3.436(7)	146
	C5–H5···O13'	0.98	2.85	3.624(7)	137
	C1'–H1'···O13	0.98	2.47	3.335(7)	147
	C3'–H3'···O13	0.98	2.56	3.384(8)	142
	C5'–H5'···O13	0.98	2.83	3.586(7)	135

Table ST2: Geometrical parameters for host-host C–H···O interactions.

	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symmetry code
1·1DCM	C2'–H2'···O7	0.98	2.68	3.467(10)	138	*x*, -1+*y*, *z*
	C8–H8*A*···O7'	0.96	2.52	3.439(13)	160	*x*, 1+*y*, *z*
	C12'–H12*D*···O13'	0.96	2.51	3.447(11)	166	1-*x*, 1/2+*y*, 1-*z*
	C12'–H12*F*···O9	0.96	2.56	3.375(13)	142	*x*, -1+*y*, *z*
	C14–H14*A*···O14	0.96	2.39	3.326(14)	166	-*x*, -1/2+*y*, 1-*z*
	C20'–H20*C*···O5	0.97	2.71	3.558(12)	147	*x*, *y*, *z*
1·2AN	C2–H2···O9'	0.98	2.70	3.485(4)	138	1+*x*, 1+*y*, 1+*z*
	C2'–H2'···O7	0.98	2.60	3.393(4)	158	-1+*x*, -1+*y*, -1+*z*
	C8–H8*A*···O7'	0.96	2.47	3.382(3)	138	1+*x*, 1+*y*, 1+*z*
	C10–H10*B*···O12'	0.96	2.67	3.509(6)	146	*x*, *y*, 1+*z*
	C12'–H12*D*···O13'	0.96	2.48	3.431(5)	169	*x*, -1+*y*, *z*
	C12'–H12*F*···O9	0.96	2.56	3.368(3)	142	-1+*x*, -1+*y*, -1+*z*
	C20–H20*B*···O8	0.97	2.68	3.386(4)	130	*x*, -1+*y*, *z*
	C26'–H26*E*···O14	0.96	2.61	3.515(4)	158	*x*, 1+*y*, *z*
1·2NM	C2–H2···O9'	0.98	2.72	3.511(9)	138	1+*x*, 1+*y*, 1+*z*
	C2'–H2'···O7	0.98	2.59	3.388(1)	139	-1+*x*, -1+*y*, -1+*z*
	C8–H8*A*···O7'	0.96	2.52	3.386(7)	151	1+*x*, 1+*y*, 1+*z*
	C10–H10*B*···O12'	0.96	2.80	3.594(8)	141	*x*, *y*, 1+*z*
	C12'–H12*D*···O13'	0.96	2.89	3.414(7)	115	-1+*x*, -1+*y*, -1+*z*
	C12'–H12*F*···O9	0.96	2.49	3.363(7)	151	*x*, -1+*y*, *z*
	C20–H20*B*···O8	0.97	2.69	3.411(10)	132	*x*, -1+*y*, *z*
	C26'–H26*E*···O14	0.96	2.61	3.520(10)	159	*x*, 1+*y*, *z*
1·2AC	C8–H8*B*···O11'	0.96	2.46	3.365(1)	156	*x*, -1+*y*, *z*

	C12–H12*A*···O14'	0.96	2.52	3.360(1)	146	-1+*x*, *y*, *z*
	C12'–H12*F*···O11	0.96	2.59	3.405(1)	143	*x*, 1+*y*, *z*
	C20–H20*A*···O12	0.97	2.83	3.705(1)	150	-*x*, 1/2+*y*, -*z*
	C21'–H21'···O12'	0.98	2.39	3.304(1)	155	-1+*x*, -1/2+*y*, 1-*z*
	C22–H22*A*···O8'	0.97	2.62	3.553(1)	161	*x*, 1+*y*, *z*
	C22–H22*B*···O12	0.97	2.51	3.449(1)	163	-*x*, -1/2+*y*, 1-*z*
1·2CF	C8–H8*B*···O11'	0.96	2.47	3.429(6)	175	*x*, -1+*y*, *z*
	C12–H12*A*···O14'	0.96	3.11	3.523(6)	108	-1+*x*, *y*, *z*
	C12'–H12*F*···O11	0.96	2.40	3.350(9)	168	*x*, 1+*y*, *z*
	C20–H20*A*···O12	0.97	2.60	3.444(12)	146	-*x*, 1/2+*y*, -*z*
	C21'–H21'···O12'	0.98	2.42	3.273(9)	146	-1+*x*, -1/2+*y*, 1-*z*
	C22–H22*A*···O8'	0.97	2.69	3.640(9)	166	*x*, 1+*y*, *z*
	C22–H22*B*···O12	0.97	2.53	3.398(9)	149	-*x*, -1/2+*y*, 1-*z*
1·2DCE	C8–H8*B*···O11'	0.96	2.47	3.426(8)	176	*x*, -1+*y*, *z*
	C12–H12*A*···O14'	0.96	2.51	3.386(8)	151	-1+*x*, *y*, *z*
	C12'–H12*F*···O11	0.96	2.47	3.382(9)	159	x, 1+y, z
	C20–H20*A*···O12	0.97	2.86	3.510(9)	125	-*x*, 1/2+*y*, -*z*
	C21'–H21'···O12'	0.98	2.44	3.308(8)	147	-1+*x*, -1/2+*y*, 1-*z*
	C22–H22*A*···O8'	0.97	2.66	3.613(8)	167	*x*, 1+*y*, *z*
	C22–H22*B*···O12	0.97	2.81	3.732(9)	160	-*x*, -1/2+*y*, 1-*z*
1·2DCM	C8–H8*B*···O11'	0.96	2.41	3.361(11)	169	*x*, -1+*y*, *z*
	C12–H12*A*···O14'	0.96	2.40	3.347(9)	168	-1+*x*, *y*, *z*
	C12'–H12*F*···O11	0.96	2.47	3.382(9)	159	*x*, 1+*y*, *z*
	C20–H20*A*···O12	0.97	2.55	3.396(20)	146	-*x*, 1/2+*y*, -*z*
	C21'–H21'···O12'	0.98	2.42	3.297(8)	149	-1+*x*, -1/2+*y*, 1-*z*

	C22–H22*A*··O8'	0.97	2.63	3.549(11)	158	*x*, 1+*y*, *z*
	C22–H22*B*··O12	0.97	2.56	3.409(10)	146	-*x*, -1/2+*y*, 1-*z*

Table ST3: Geometrical parameters for significant host-guest interactions.

	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symmetry code
1·1DCM	C10–H10*C*···Cl2	0.96	2.81	3.718(18)	157	-1+*x*, 1+*y*, *z*
	C16–H16*C*···Cl2	0.96	2.95	3.520(18)	119	*x*, *y*, *z*
	C17–H17*A*···Cl1	0.97	2.85	3.815(12)	173	-1+*x*, 1+*y*, *z*
	C22'–H22*D*···Cl2	0.97	2.83	3.698(22)	149	*x*, *y*, *z*
	C27–H27*A*···O14	0.97	2.23	3.109(31)	151	-1+*x*, 1+*y*, *z*
	$^{\Psi}$C27–Cl1···O12'	-	3.136(12)	-	158.4(6)	*x*, 1+*y*, *z*
1·2AN	C10–H10*C*···O1*W*	0.96	2.58	3.439(10)	149	*x*, *y*, *z*
	C14–H14*C*···N2	0.96	2.66	3.563(9)	157	*x*, 1+*y*, 1+*z*
	C16'–H16*D*···N1	0.96	2.74	3.460(8)	132	-1+*x*, *y*, -1+*z*
	C17–H17*A*···O1*W*	0.97	2.55	3.453(10)	156	*x*, *y*, *z*
	C27–H27*A*···O8	0.96	2.55	3.451(4)	158	1+*x*, *y*, *z*
	C27–H27*B*···O7'	0.96	2.63	3.314(6)	128	1+*x*, *y*, *z*
	C30–H30*B*···O11	0.96	2.70	3.385(7)	129	*x*, -1+*y*, -1+*z*
1·2NM	C8–H8*A*···O16	0.96	2.68	3.292(45)	122	1+*x*, 1+*y*, *z*
	C10'–H10*D*···O18	0.96	2.63	3.543(18)	168	*x*, *y*, *z*
	C14–H14*C*···O18	0.96	2.60	3.317(28)	131	*x*, *y*, *z*
	C16–H16*A*···O16	0.96	2.47	3.362(60)	155	1+*x*, 1+*y*, *z*
	C16–H16*C*···O17	0.97	2.63	3.433(27)	142	*x*, *y*, *z*
	C17–H17*A*···O1*W*	0.97	2.59	3.484(31)	154	*x*, *y*, *z*
	C27–H27*B*···O7'	0.96	2.49	3.181(15)	129	*x*, *y*, *z*
	C28–H28*A*···O11	0.96	2.59	3.277(15)	129	*x*, *y*, *z*
1·2AC	C16'–H16*F*···O16	0.96	2.74	3.368(11)	123	*x*, *y*, *z*
	C16–H16*C*···O15’	0.96	2.61	3.438(1)	144	-1+*x*, *y*, *z*

1·2CF	C2'–H2'···Cl5	0.98	2.89	3.656(6)	136	1-*x*, 1/2+*y*, 1-*z*
	C8–H8*C*···Cl3	0.96	2.95	3.821(7)	152	-1+*x*, 1+*y*, *z*
	C8'–H8*F*···Cl4	0.96	2.72	3.673(11)	170	*x*, 1+*y*, *z*
	C10'–H10*F*···Cl1	0.96	2.75	3.415(22)	128	*x*, *y*, *z*
	C12'–H12*E*···Cl5	0.96	2.66	3.373(9)	131	*x*, *y*, *z*
	C16'–H16*E*···Cl1	0.96	2.85	3.791(7)	167	-1+*x*, *y*, *z*
	C27–H27···O7	0.98	2.34	3.159(9)	140	1-*x*, -1/2+*y*, -*z*
	C28–H28···O9'	0.98	2.42	3.132(15)	129	1-*x*, -1/2+*y*, 1-*z*
	[Ψ]C27–Cl3···O9	-	2.845(5)	-	166.6(3)	1-*x*, 1/2+*y*, 1-*z*
	[Ψ]C28–Cl5···O7'	-	2.688(6)	-	157.8(4)	1-*x*, -1/2+*y*, 1-*z*
1·2DCE	C10'–H10*E*···Cl3	0.96	2.95	3.638(9)	130	1-*x*, -1/2+*y*, 1-*z*
	C16–H16*C*···Cl2	0.96	2.78	3.711(7)	163	-1+*x*, *y*, *z*
	C26–H26*D*···Cl3	0.96	2.91	3.860(9)	169	-1+*x*, *y*, *z*
	C27–H27*B*···O13	0.97	2.67	3.311(9)	124	1-*x*, 1/2+*y*, 1-*z*
	C28–H28*B*···O13	0.97	2.67	3.054(8)	104	1-*x*, 1/2+*y*, 1-*z*
	C28–H28*B*···O14	0.97	2.65	3.317(9)	126	1-*x*, 1/2+*y*, 1-*z*
	C29–H29*B*···O12'	0.97	2.62	3.550(9)	160	1-*x*, -1/2+*y*, -*z*
1·2DCM	C27–H27*A*···O7	0.97	2.65	3.267(13)	121	*x*, *y*, *z*
	C27–H27*B*···O9	0.97	2.71	3.680(11)	176	*x*, *y*, *z*
	C28–H28*A*···O9'	0.97	2.67	3.316(13)	125	*x*, *y*, 1+*z*

[Ψ] Halogen bonding contacts