

**Supplementary Information for the paper :**

**Similarities and Differences Between Molecular Order in the Nematic and Twist-bend Nematic Phases of a Symmetric Liquid Crystal Dimer**

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Table S1. The differences,  $\Delta_i$  /ppm for <sup>13</sup>C nuclei in DTC5C9. The values of  $\delta_i$  were taken from a spectrum recorded in the isotropic phase at 166 °C.

T / °C	Carbon site						
	1 or 13	13 or 1	2 and 5	3 or 4	4 or 3	8,12	9,11
158	36.208	36.208	26.857	11.150	11.150	12.610	12.610
156	39.028	39.028	27.407	11.960	11.960	13.584	13.584
154	41.138	41.138	28.807	12.550	12.550	14.306	14.306
152	42.788	42.788	29.827	13.050	13.050	14.867	14.867
150	43.598	44.468	30.727	13.380	13.380	15.067	15.067

148	44.748	45.218	31.517	13.610	13.610	15.347	15.347
146	45.598	46.048	32.167	13.941	13.767	15.667	15.667
144	46.348	46.848	32.647	14.150	13.950	16.327	16.327
142		47.568	33.057	14.331	14.102	16.102	16.102
141	47.232	47.703	33.257	14.405	14.164	16.187	16.187
140	47.468	47.948	33.397	14.455	14.217	16.266	16.266
139	47.718	48.238	33.577	14.511	14.267	16.327	16.327
138	47.898	48.398	33.697	14.548	14.306	16.388	16.388
137	48.048	48.558	33.741	14.572	14.325	16.427	16.427
136	48.169	48.649	33.807	14.599	14.353	16.463	16.463
135	48.219	48.695	33.817	14.597	14.350	16.480	16.480
134	48.237	48.714	33.807	14.592	14.344	16.480	16.480
134	48.175	48.611	33.727	14.515	14.272	16.417	16.417
132	48.148	48.628	33.737	14.539	14.283	16.422	16.422
130	47.668	48.258	33.337	14.361	14.103	16.267	16.267
128	47.248	47.828	32.967	14.252	13.996	16.151	16.151
124	46.538	47.058	32.387	13.951	13.715	15.889	15.889
122	46.062	46.561	32.127	13.789	13.551	15.723	15.723
120	45.728	46.242	31.787	13.658	13.434	15.604	15.604
118	45.464	45.961	31.567	13.547	13.323	15.501	15.501
116	45.223	45.743	31.547	13.453	13.236	15.419	15.419
114	45.039	45.525	31.387	13.363	13.159	15.337	15.337
112	44.859	45.356	31.227	13.289	13.093	15.279	15.279
110	44.762	45.193	31.107	13.222	13.035	15.211	15.211
108	44.619	45.033	30.967	13.154	12.974	15.151	15.151

106	44.439	44.885	30.867	13.095	12.927	15.097	15.097
104	44.153	44.612	30.597	12.900	12.731	14.895	14.895
102	44.235	44.643	30.657	12.954	12.839	14.993	14.993
100	44.148	44.519	30.587	12.915	12.832	14.957	14.957
98	43.960	44.422	30.487	12.812	12.812	14.913	14.913
96	43.926	44.334	30.407	12.785	12.785	14.874	14.874
95	43.264	44.209	30.327	12.776	12.776	14.867	14.867
94	43.896			12.769	12.769	14.846	14.846
93	43.858	44.261	30.377	12.765	12.765	14.846	14.846
92	43.862	44.266	30.347	12.760	12.760	14.846	14.846
91	43.896	44.289	30.287	12.764	12.764	14.852	14.852
90	43.988	44.338	30.327	12.764	12.764	14.876	14.876
89	44.112	44.452	30.397	12.905	12.728	14.924	14.924
88	44.377	44.696	30.597	13.015	12.761	15.020	15.020
87			31.077	13.299	12.846	15.246	15.246
86	47.418	47.798	32.537			16.041	16.041
85			33.317	14.710	13.360	16.467	16.467
84	48.998	49.358		15.040	13.430	16.717	16.717

Table S1 (contd)

		Carbon site					
T / °C	10 or 16	16 or 10	14,18	15,17	39	40	

158	35.632	35.632	12.387	12.387	-1.343	-1.418
156	38.472	38.472	13.361	13.361	-1.403	-1.548
154	40.532	39.762	14.083	14.083	-1.483	-1.618
152	42.072	41.422	14.344	14.344	-1.573	-1.688
150	43.442	42.692	15.144	15.144	-1.583	-1.818
148	44.502	43.762	15.504	15.504	-1.643	-1.858
146	45.502	44.672	15.854	15.854	-1.703	-1.908
144	46.182	45.292	15.694	15.694	-1.783	-2.018
142	46.882	45.902	16.296	16.296	-1.803	-2.058
141	47.112	45.972	16.374	16.374	-1.806	-2.063
140	47.362	46.242	16.451	16.451	-1.817	-2.098
139	47.682	46.472	16.579	16.511	-1.824	-2.110
138	47.892	46.692	16.647	16.546	-1.827	-2.118
137	48.032	46.802	16.697	16.697	-1.833	-2.138
136	48.107	46.884	16.742	16.615	-1.843	-2.158
135	48.150	46.933	16.760	16.628	-1.834	-2.158
134	48.166	46.945	16.788	16.632	-1.853	-2.170
134	48.098	46.876	16.703	16.548		

132	48.104	46.853	16.732	16.591	-1.905	-2.228
130	47.732	46.482	16.544	16.432	-1.834	-2.175
128	47.302	46.072	16.419	16.331	-1.871	-2.227
124	47.352	45.362	16.157	16.045	-1.803	-2.168
122	46.092	44.872	15.992	15.880		
120	45.772	44.542	15.840	15.746		
118	45.502	44.242	15.732	15.641	-1.777	-2.181
116	45.270	44.009	15.638	15.553	-1.764	-2.183
114	45.071	43.817	15.568	15.479	-1.747	-2.184
112	44.896	43.544	15.387	15.414	-1.737	-2.190
110	44.723	43.456	15.448	15.358	-1.730	-2.202
108	44.577	43.304	15.388	15.300	-1.721	-2.210
106	44.435	43.152	15.313	15.243	-1.715	-2.223
104	44.161	42.859	15.140	15.046	-1.708	-2.235
102	44.232	42.925	15.233	15.142	-1.698	-2.247
100	44.082	42.772	15.193	15.101	-1.695	-2.261
98	43.976	42.652	15.063	15.063	-1.841	-2.424
96	43.894	42.567	15.034	15.034	-1.680	-2.282

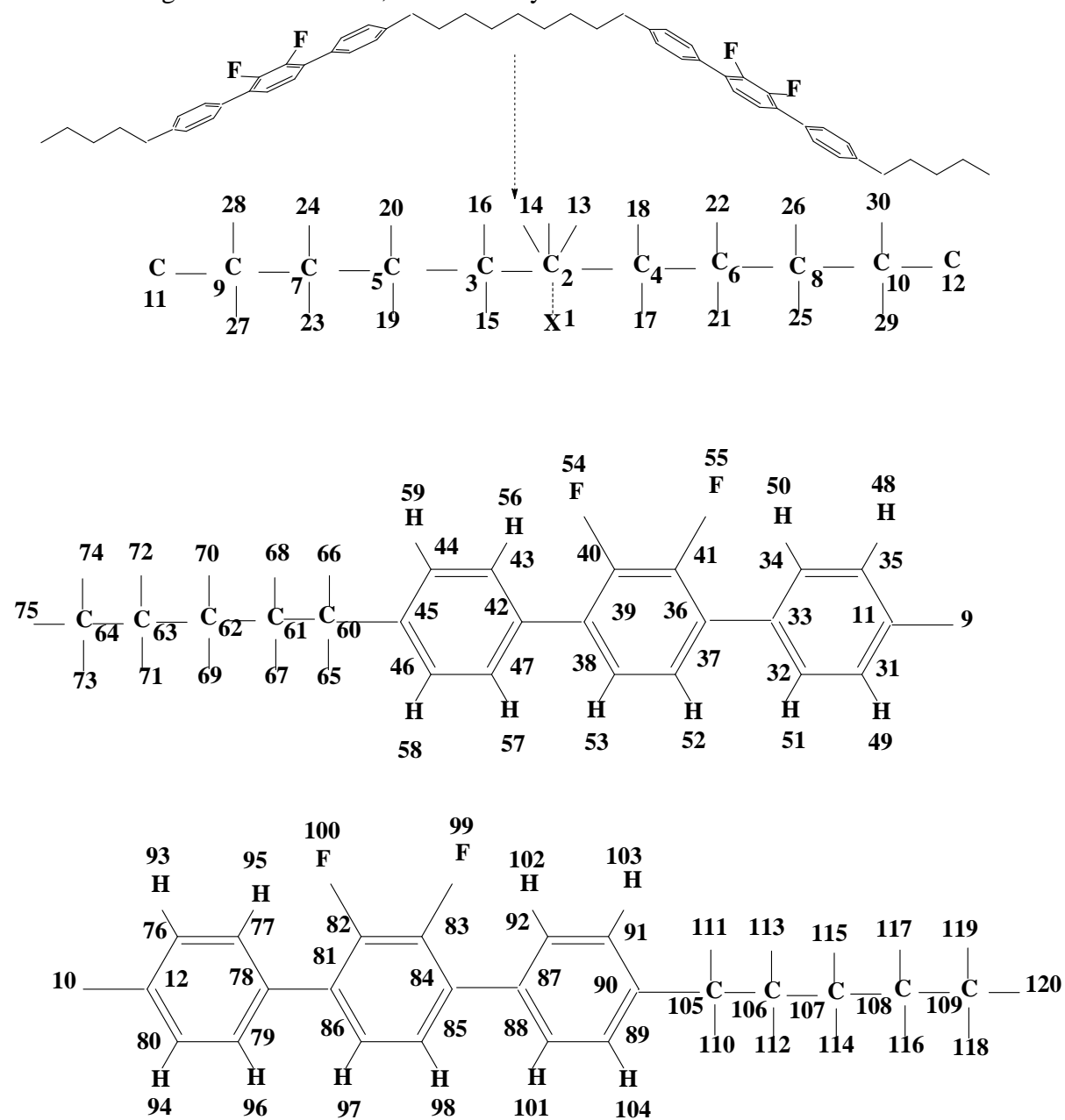
95	43.852	42.531	15.015	15.015	-1.674	-2.297
94	43.828	42.503	14.995	14.971	-1.667	-2.309
93	43.816	42.483	15.085	14.968	-1.662	-2.326
92	43.748	42.487	15.078	14.971	-1.657	-2.335
91	43.864	42.509	15.076	14.971	-1.655	-2.339
90	43.876	42.568	15.088	14.988	-1.653	-2.347
89	43.992	42.682	15.121	15.024	-1.649	-2.360
88	44.224	42.956	15.195	15.108	-1.646	-2.367
87	44.892	43.692	15.396	15.311	-1.643	-2.381
86	46.852	45.972	16.034	16.034	-1.647	-2.399
85	47.952	46.992	16.434	16.434	-1.656	-2.432
84	48.582	46.742	16.644	16.644	-1.685	-2.493

Table S2. The average of the C-F total couplings for resolved  $^{13}\text{C}$  resonances in the  $^{13}\text{C}$  –  $\{^1\text{H}\}$  spectra of Mehl compound.

T/ °C	Average $D_{\text{CF}}$ for each ring carbon/Hz											
	1 or 13	2 or 5	3 or 4	4 or 3	5 or 2	8 or 14	9 or 15	10 or 16	13 or 1	14 or 8	15 or 9	16 or 10
158	0	0	0	53	0	0	0	0	0	0	0	0
156	0	0	0	58	0	0	0	0	0	0	0	0
154	0	158	0	64	158	0	0	0	0	0	0	0
152	0	165.5	0	68.5	165.5	0	0	0	0	0	0	0
150	0	168.5	0	72.5	168.5	0	0	0	0	0	0	0
148	0	176.5	0	72	176.5	0	0	0	0	0	0	0
146	0	178.5	74.5	74.5	178.5	0	0	0	0	0	0	0
144	30	182.5	75	75	182.5	97	61	0	0	95	60	0

142	37.5	185.5	76.5	77	185.5	97.5	62.5	0	0	95	61	0
141	0	183	77	77	183	99	62	50	0	96	62	47.5
140	0	188	77.5	78	188	100	62.5	55	0	96.5	62	45
139	38	188	78	78.5	188	98.5	63.5	50	30.5	98	62.5	47
138	37	188.5	78.5	78.5	188.5	100	64	47.5	30	97	62.5	47.5
137	37	191	79	79	191	101	64	50	33	97.5	62.5	50
136	36	189	79	79.5	189	100.5	64.5	50.5	34.5	99	63	49
135	36	191.5	78.5	79.5	191.5	100.5	64.5	50.5	34.5	98	63	49.5
134	36.5	193	78.5	79.5	193	101	64	50	33.5	99.5	63	50
132	38	192	79	79.5	192	101	64.5	50	34.5	99	63	49.5
130	37.5	193.5	79	79.5	193.5	101	64.5	50.5	33.5	99	63	49.5
128	35	193	79	79	193	100	62	50	0	98	63	48.5
124	34.5	195	78	78.5	195	99.5	62.5	49	35	96.5	62	50.5
118	34.5	190	77.5	78	190	98	62.5	48	0	98.5	60	48
116	33	188	77	77.5	188	97.5	62	49	31	94	60.5	47.5
114	31	191.5	77	77	191.5	96.5	61.5	46.5	30	93	60.5	49
112	35	190	76.5	77	190	96	62	47	27.5	92.5	59.5	48.5
110	30.5	186.5	76	76.5	186.5	96	61	46	25.5	92.5	59.5	47.5
108	34	188.5	76.5	76.5	188.5	95	59	46.5	25.5	93	59	48
106	30	181.5	76	76.5	181.5	95	60	47	26.5	91.5	59	46.5
104	31.5	181.5	76.5	76	181.5	95	61	46	31	91.5	59	46.5
102	31.5	181.5	76	76	181.5	95	60	46.5	31	92	58.5	46
100	31.5	181.5	75.5	76	181.5	94	60	47.5	31	91.5	58	46
98	32	181.5	75.5	76	181.5	94	60	47	0	91.5	58.5	46
96	31	180.5	75.5	75.5	180.5	93.5	60	46	31	91	58.5	46
95	31.5	180	75.5	75.5	180	93.5	59	45.5	31.5	91.5	58.5	46.5
94	31.5	180	75.5	75.5	180	93.5	60	45	27	91.5	58	45.5
93	30	180	75.5	75.5	180	93	62	45.5	28	91.5	58.5	45
92	31	181.5	75	75	181.5	93	59	46	27.5	91	58.5	46
91	31	189.5	76	76	189.5	93	59	46	30	91.5	58.5	46
90	30	189.5	76	76	189.5	93	59	46	29.5	91	56.5	45.5
89	29	186	76	76	186	93	59	46.5	29	91.5	59	45.5
88	30	186	76	76	186	93	59	45.5	30	91.5	59	46
87	29.5	185	76	76	185	93	58.5	46	31	92.5	59	45.5
86	29.5	187	76	77	187	93	58.5	46	32	93.5	59	45
85	26.5	183	76.5	77	183	93.5	58.5	45	32.5	93	60	46
86	0	190	78	78.5	190	94.5	59	47.5	0	98.5		44

Table S3. The bond lengths,  $r_{ij}$ , the bond angles,  $\theta_{ijk}$ , and dihedral angles,  $\delta_{ijks}$ , of DTC5C9 in the most elongated conformation, calculated by the DFT method<sup>1</sup> B3LYP/6-31G\*.



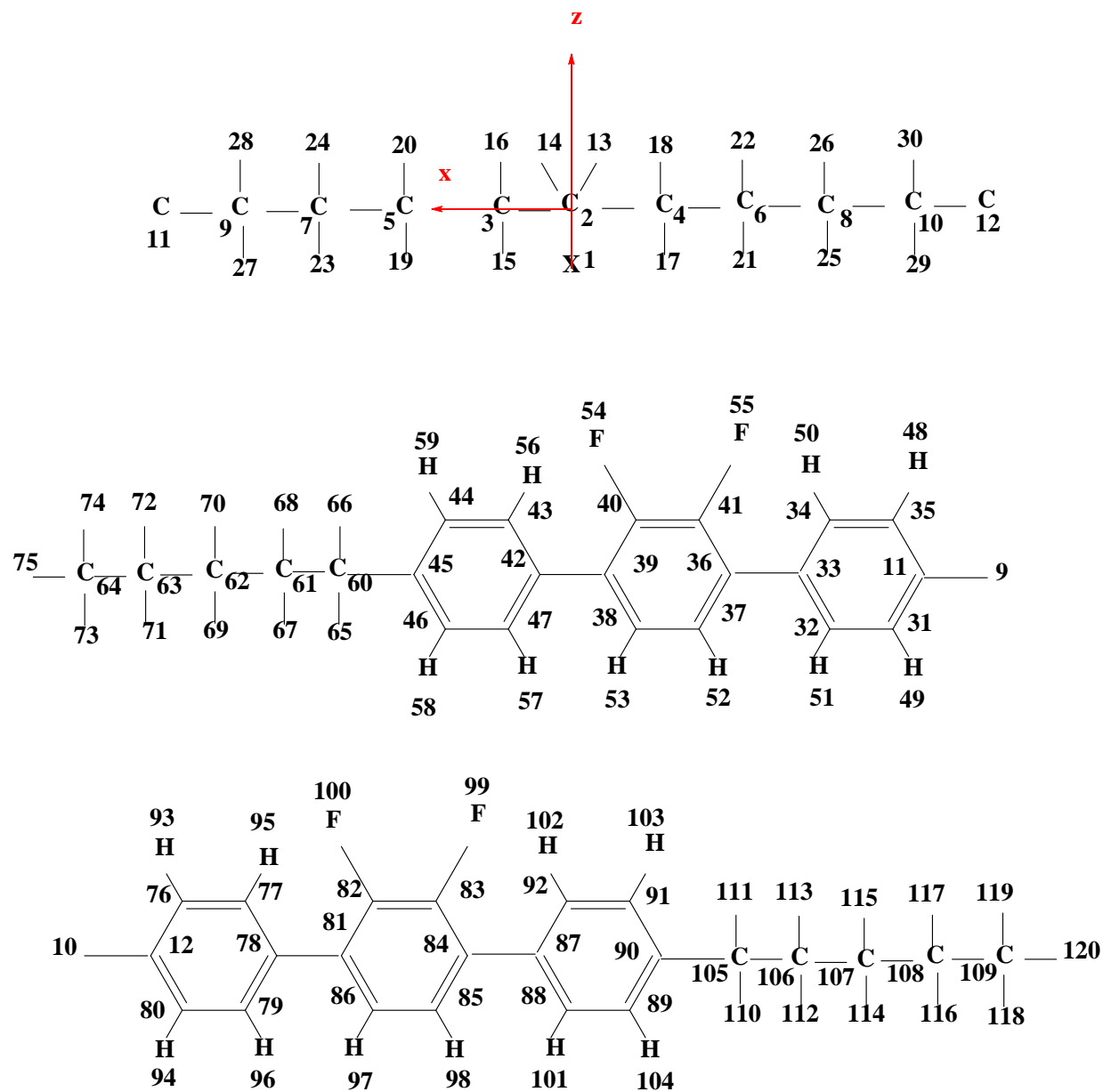


<i>i</i>	<i>j</i>	$r_{ij}/\text{\AA}$	<i>k</i>	$\theta_{i,j,k}/^\circ$	<i>s</i>	$\delta_{I,j,k,s}/^\circ$
1	X					
2	C	1				
3	C	2	1	123.2		
4	C	2	1	123.2	3	180.0*
5	C	3	2	113.3	4	180.0
6	C	4	2	113.3	3	180.5
7	C	5	3	113.6	2	179.8
8	C	6	4	113.6	2	181.1
9	C	7	5	113.0	3	179.9
10	C	8	6	113.0	4	180.9
11	C	9	7	113.2	5	179.5
12	C	10	8	113.2	6	181.0
13	H	2	3	109.2	4	122.3
14	H	2	3	109.2	4	-122.3
15	H	3	2	109.3	5	122.2
16	H	3	2	109.3	5	-122.2
17	H	4	2	109.3	6	122.2
18	H	4	2	109.3	6	-122.2
19	H	5	3	109.3	7	122.3
20	H	5	3	109.3	7	-122.2
21	H	6	4	109.3	8	122.2
22	H	6	4	109.3	8	-122.3
23	H	7	5	109.7	9	121.9
24	H	7	5	109.7	9	-122.0
25	H	8	6	109.7	10	121.9
26	H	8	6	109.7	10	-121.9
27	H	9	7	108.9	11	122.2
28	H	9	7	108.9	11	-122.1
29	H	10	8	108.9	12	122.1
30	H	10	8	108.9	12	-122.2
31	C	11	9	121.2	7	89.0
32	C	31	11	121.2	9	181.8
33	C	32	31	121.1	11	-0.1
34	C	33	32	117.8	31	0.4
35	C	34	33	120.8	32	-0.5
36	C	33	32	120.1	31	181.9
37	C	36	33	121.6	32	37.1
38	C	37	36	122.0	33	180.4
39	C	38	37	122.0	36	0.0
40	C	39	38	115.9	37	0.0
41	C	40	39	122.1	38	0.0
42	C	39	40	122.6	41	180.2
43	C	42	39	120.1	40	142.3
44	C	43	42	121.1	39	178.4
45	C	44	43	121.2	42	0.1

46	C	45	1.401	44	117.7	43	0.3
47	C	46	1.392	45	121.5	44	-0.2
48	H	35	1.088	11	119.4	31	179.5
49	H	31	1.088	11	119.5	35	179.7
50	H	34	1.084	33	119.7	32	180.4
51	H	32	1.087	33	119.5	34	181.4
52	H	37	1.085	36	118.6	41	182.3
53	H	38	1.085	39	118.6	40	177.7
54	F	40	1.349	39	120.9	38	178.7
55	F	41	1.349	36	120.9	37	181.3
56	H	43	1.087	42	119.5	47	177.9
57	H	47	1.084	42	119.7	43	180.2
58	H	46	1.088	45	119.4	44	179.8
59	H	44	1.088	45	119.5	46	181.0
60	C	45	1.513	44	121.2	43	181.9
61	C	60	1.543	45	113.0	44	89.9
62	C	61	1.534	60	113.1	45	179.7
63	C	62	1.534	61	113.4	60	180.0
64	C	63	1.532	62	113.2	61	179.9
65	H	60	1.098	45	109.6	61	121.7
66	H	60	1.098	45	109.7	61	-121.8
67	H	61	1.099	60	109.0	62	122.4
68	H	61	1.099	60	109.0	62	-122.3
69	H	62	1.100	61	109.3	63	122.2
70	H	62	1.100	61	109.4	63	-122.2
71	H	63	1.099	62	109.2	64	122.2
72	H	63	1.099	62	109.2	64	-122.2
73	H	64	1.096	63	111.4	62	179.9
74	H	64	1.097	63	111.2	73	120.1
75	H	64	1.097	63	111.2	73	-120.1
76	C	12	1.401	10	121.2	8	92.4
77	C	76	1.392	12	121.5	10	181.1
78	C	77	1.405	76	120.8	12	0.3
79	C	78	1.405	77	117.8	76	-0.3
80	C	79	1.392	78	121.1	77	0.2
81	C	78	1.483	77	122.1	76	178.9
82	C	81	1.399	78	122.6	77	38.9
83	C	82	1.392	81	122.2	78	179.2
84	C	83	1.399	82	122.1	81	0.0
85	C	84	1.407	83	115.8	82	0.2
86	C	85	1.389	84	122.0	83	-0.2
87	C	84	1.483	85	121.6	86	179.2
88	C	87	1.405	84	122.1	85	142.0
89	C	88	1.392	87	120.8	84	181.0
90	C	89	1.401	88	121.5	87	-0.2
91	C	90	1.401	89	117.7	88	0.0

92	C	91	1.393	90	121.2	89	0.1
93	H	76	1.088	12	119.4	80	180.2
94	H	80	1.088	12	119.5	76	179.0
95	H	77	1.084	78	119.7	79	179.9
96	H	79	1.087	78	119.5	77	182.0
97	H	86	1.085	81	118.6	82	182.3
98	H	85	1.085	84	118.6	83	177.7
99	F	83	1.349	84	120.9	85	178.8
100	F	82	1.349	81	120.9	86	181.3
101	H	88	1.084	87	119.7	92	180.1
102	H	92	1.087	87	119.5	88	178.0
103	H	91	1.088	90	119.5	89	181.0
104	H	89	1.088	90	119.4	91	179.8
105	C	90	1.513	91	121.2	92	181.4
106	C	105	1.543	90	113.2	91	89.2
107	C	106	1.533	105	113.1	90	179.7
108	C	107	1.534	106	113.5	105	180.0
109	C	108	1.532	107	113.2	106	179.9
110	H	105	1.098	90	109.6	106	121.7
111	H	105	1.098	90	109.6	106	-121.8
112	H	106	1.099	105	109.0	107	122.3
113	H	106	1.099	105	109.1	107	-122.3
114	H	107	1.100	106	109.3	108	122.2
115	H	107	1.100	106	109.4	108	-122.2
116	H	108	1.099	107	109.2	109	122.2
117	H	108	1.099	107	109.2	109	-122.2
118	H	109	1.096	108	111.4	107	179.9
119	H	109	1.097	108	111.2	118	120.1
120	H	109	1.097	108	111.2	118	-120.1

Table S4. Nuclear magnetic shielding tensor components (ppm) for DTC5C9 calculated by a DFT method using a B3LYP functional and a 6-31G\* basis set.



2 C Isotropic = 156.1583 Anisotropy = 33.0943  
 XX= 178.2208 YX= 0.0042 ZX= -0.1354  
 XY= -0.0986 YY= 137.6753 ZY= -0.2054  
 XZ= -0.0049 YZ= -0.0988 ZZ= 152.5786  
 Eigenvalues: 137.6737 152.5799 178.2211

3 C Isotropic = 156.3285 Anisotropy = 32.6830  
 XX= 178.1147 YX= 0.0196 ZX= 0.1669  
 XY= 0.1113 YY= 137.8292 ZY= -0.1243  
 XZ= 0.3299 YZ= -0.0746 ZZ= 153.0418  
 Eigenvalues: 137.8284 153.0400 178.1172

4 C Isotropic = 156.3820 Anisotropy = 32.7552  
 XX= 178.2168 YX= -0.0772 ZX= -0.1355  
 XY= 0.2414 YY= 137.9071 ZY= -0.1173  
 XZ= -0.2924 YZ= -0.0113 ZZ= 153.0220  
 Eigenvalues: 137.9066 153.0205 178.2188

5 C Isotropic = 155.7537 Anisotropy = 33.3117  
 XX= 177.9474 YX= -0.0150 ZX= 0.7245  
 XY= 0.1473 YY= 138.0288 ZY= -0.0662  
 XZ= 0.4992 YZ= -0.0011 ZZ= 151.2850  
 Eigenvalues: 138.0286 151.2711 177.9616

6 C Isotropic = 155.8031 Anisotropy = 33.2625  
 XX= 177.9609 YX= -0.1060 ZX= -0.7196  
 XY= -0.4317 YY= 138.0868 ZY= -0.1300  
 XZ= -0.5593 YZ= -0.0017 ZZ= 151.3616  
 Eigenvalues: 138.0846 151.3466 177.9781

7 C Isotropic = 152.1108 Anisotropy = 40.8675  
 XX= 179.1520 YX= 0.0750 ZX= 6.0817  
 XY= 0.0466 YY= 133.6312 ZY= 0.1618  
 XZ= -0.6808 YZ= 0.1920 ZZ= 143.5491  
 Eigenvalues: 133.6281 143.3485 179.3558

8 C Isotropic = 152.1465 Anisotropy = 40.7247  
 XX= 179.0822 YX= -0.6390 ZX= -6.0689  
 XY= 0.6272 YY= 133.5860 ZY= -0.5418  
 XZ= 0.5535 YZ= -0.2562 ZZ= 143.7714  
 Eigenvalues: 133.5701 143.5732 179.2963

9 C Isotropic = 150.3029 Anisotropy = 33.1360  
 XX= 167.3953 YX= 0.2717 ZX= 20.1774  
 XY= 0.1624 YY= 138.4850 ZY= 0.2539  
 XZ= 3.2095 YZ= -0.1962 ZZ= 145.0284  
 Eigenvalues: 138.4814 140.0337 172.3936

10 C Isotropic = 150.2693 Anisotropy = 33.3180  
 XX= 167.4577 YX= -0.8860 ZX= -20.1552  
 XY= -0.7670 YY= 138.4394 ZY= -0.5017  
 XZ= -3.3562 YZ= -0.4894 ZZ= 144.9109  
 Eigenvalues: 138.0927 140.2339 172.4813

11 C Isotropic = 53.2371 Anisotropy = 185.8862  
 XX= 38.9250 YX= -0.4425 ZX= -96.0866  
 XY= -0.4220 YY= 12.7605 ZY= 1.0288  
 XZ= -99.4334 YZ= -1.8792 ZZ= 108.0258  
 Eigenvalues: -30.2187 12.7688 177.1613

12 C Isotropic = 53.3052 Anisotropy = 185.6519  
 XX= 36.1756 YX= 11.3883 ZX= 96.8159  
 XY= 8.9945 YY= 14.3573 ZY= 11.7315  
 XZ= 95.2807 YZ= 12.2602 ZZ= 109.3827  
 Eigenvalues: -30.0656 12.9081 177.0731

13 H Isotropic = 30.6885 Anisotropy = 3.8795  
 XX= 33.2731 YX= -0.0267 ZX= -0.0055  
 XY= 0.0008 YY= 29.3905 ZY= -3.4282  
 XZ= 0.0107 YZ= -4.1915 ZZ= 29.4020  
 Eigenvalues: 25.5864 33.2043 33.2749

14 H Isotropic = 30.6931 Anisotropy = 3.9251  
 XX= 33.3089 YX= -0.0497 ZX= 0.0164  
 XY= 0.0072 YY= 29.3684 ZY= 3.3709  
 XZ= -0.0091 YZ= 4.1646 ZZ= 29.4021  
 Eigenvalues: 25.6175 33.1520 33.3099

15 H Isotropic = 30.7282 Anisotropy = 4.3899  
 XX= 33.6476 YX= -0.0179 ZX= 0.2006  
 XY= 0.1099 YY= 29.3283 ZY= 3.3454  
 XZ= -0.1144 YZ= 4.3313 ZZ= 29.2088  
 Eigenvalues: 25.4297 33.1001 33.6548

16 H Isotropic = 30.7427 Anisotropy = 4.3395  
 XX= 33.6341 YX= -0.0161 ZX= 0.1919  
 XY= -0.0169 YY= 29.3601 ZY= -3.3341  
 XZ= -0.1431 YZ= -4.3192 ZZ= 29.2340  
 Eigenvalues: 25.4699 33.1226 33.6357

17 H Isotropic = 30.7376 Anisotropy = 4.3114  
 XX= 33.6101 YX= -0.0463 ZX= -0.1319  
 XY= 0.1138 YY= 29.3037 ZY= -3.4041  
 XZ= 0.1250 YZ= -4.3649 ZZ= 29.2989  
 Eigenvalues: 25.4167 33.1842 33.6118

18 H Isotropic = 30.7326 Anisotropy = 4.4100  
 XX= 33.6680 YX= -0.0353 ZX= -0.2237  
 XY= -0.0090 YY= 29.3845 ZY= 3.2820  
 XZ= 0.1163 YZ= 4.2751 ZZ= 29.1454  
 Eigenvalues: 25.4844 33.0408 33.6726

19 H Isotropic = 30.6251 Anisotropy = 3.9308  
 XX= 33.1589 YX= -0.0673 ZX= 0.4338  
 XY= -0.2422 YY= 29.5516 ZY= 3.3344  
 XZ= 0.1869 YZ= 4.1454 ZZ= 29.1648  
 Eigenvalues: 25.5987 33.0309 33.2456

20 H Isotropic = 30.6216 Anisotropy = 3.9602  
 XX= 33.1521 YX= 0.0344 ZX= 0.4648  
 XY= 0.2463 YY= 29.5140 ZY= -3.2948  
 XZ= 0.2258 YZ= -4.1057 ZZ= 29.1986  
 Eigenvalues: 25.6367 32.9663 33.2617

21 H Isotropic = 30.6252 Anisotropy = 3.9863  
 XX= 33.1846 YX= -0.1480 ZX= -0.4917  
 XY= -0.2636 YY= 29.3489 ZY= -3.4237  
 XZ= -0.1939 YZ= -4.2135 ZZ= 29.3420  
 Eigenvalues: 25.5073 33.0855 33.2827

22 H Isotropic = 30.6132 Anisotropy = 3.9141  
 XX= 33.1330 YX= -0.0462 ZX= -0.3754  
 XY= 0.2093 YY= 29.6718 ZY= 3.2182  
 XZ= -0.1982 YZ= 4.0463 ZZ= 29.0347  
 Eigenvalues: 25.6975 32.9195 33.2226

23 H Isotropic = 30.5389 Anisotropy = 5.4790  
 XX= 33.9628 YX= 0.4293 ZX= 1.4111  
 XY= 0.6520 YY= 29.3695 ZY= 3.0394  
 XZ= -0.8009 YZ= 4.3501 ZZ= 28.2845  
 Eigenvalues: 25.0909 32.3342 34.1916

24 H Isotropic = 30.5651 Anisotropy = 5.3736  
 XX= 33.9704 YX= -0.4266 ZX= 1.3795  
 XY= -0.5601 YY= 29.3488 ZY= -2.8488  
 XZ= -0.8451 YZ= -4.2373 ZZ= 28.3761  
 Eigenvalues: 25.2844 32.2634 34.1475

25 H Isotropic = 30.5653 Anisotropy = 5.4554  
 XX= 33.9630 YX= 0.2777 ZX= -1.3537  
 XY= 0.7625 YY= 29.0787 ZY= -3.1738  
 XZ= 0.7133 YZ= -4.4757 ZZ= 28.6542  
 Eigenvalues: 25.0341 32.4597 34.2022

26 H Isotropic = 30.5761 Anisotropy = 5.3794  
 XX= 34.0045 YX= -0.5926 ZX= -1.3749  
 XY= -0.4229 YY= 29.6347 ZY= 2.6821  
 XZ= 0.9326 YZ= 4.0632 ZZ= 28.0891  
 Eigenvalues: 25.3994 32.1666 34.1624

27 H Isotropic = 29.6097 Anisotropy = 4.3812  
 XX= 30.3852 YX= -1.0539 ZX= 0.6254  
 XY= -2.1478 YY= 29.3172 ZY= 2.6150  
 XZ= 1.9034 YZ= 3.9053 ZZ= 29.1266  
 Eigenvalues: 25.1741 31.1245 32.5305

28 H Isotropic = 29.6173 Anisotropy = 4.1799  
 XX= 30.3320 YX= 0.9921 ZX= 0.6198  
 XY= 2.0562 YY= 29.1836 ZY= -2.4555  
 XZ= 1.9722 YZ= -3.8043 ZZ= 29.3363  
 Eigenvalues: 25.3319 31.1161 32.4039

29 H Isotropic = 29.6373 Anisotropy = 4.4453  
 XX= 30.5629 YX= -1.1877 ZX= -0.6480  
 XY= -2.4261 YY= 28.8956 ZY= -2.6457  
 XZ= -1.6836 YZ= -3.9898 ZZ= 29.4532  
 Eigenvalues: 25.0306 31.2804 32.6008

30 H Isotropic = 29.5767 Anisotropy = 4.1825  
 XX= 30.2043 YX= 0.8934 ZX= -0.5694  
 XY= 1.7390 YY= 29.5401 ZY= 2.4308  
 XZ= -2.1305 YZ= 3.7440 ZZ= 28.9856  
 Eigenvalues: 25.4206 30.9444 32.3650

31 C Isotropic = 67.0558 Anisotropy = 148.7177  
 XX= 76.9472 YX= -33.2185 ZX= -59.5666  
 XY= -32.6105 YY= -6.6148 ZY= -18.3581  
 XZ= -52.6259 YZ= -14.6380 ZZ= 130.8351  
 Eigenvalues: -26.4089 61.3754 166.2009

32 C Isotropic = 67.9967 Anisotropy = 151.1874  
 XX= 78.9307 YX= 19.4590 ZX= -62.6185  
 XY= 20.7672 YY= -8.5179 ZY= 20.2695  
 XZ= -48.2303 YZ= 31.1610 ZZ= 133.5774  
 Eigenvalues: -23.0917 58.2936 168.7883

33 C Isotropic = 62.0914 Anisotropy = 162.7246  
 XX= 38.9700 YX= -2.5802 ZX= -85.1231  
 XY= -0.3576 YY= 37.1418 ZY= -0.6609  
 XZ= -92.9060 YZ= 9.1209 ZZ= 110.1625  
 Eigenvalues: -21.3246 37.0244 170.5745

34 C Isotropic = 66.0595 Anisotropy = 158.9536  
 XX= 77.2364 YX= -25.4958 ZX= -63.3425  
 XY= -26.5728 YY= -10.3102 ZY= -15.1588  
 XZ= -60.7869 YZ= -9.0366 ZZ= 131.2522  
 Eigenvalues: -23.7728 49.9227 172.0285

35 C Isotropic = 67.4068 Anisotropy = 148.4550  
 XX= 75.9058 YX= 27.3015 ZX= -61.5105  
 XY= 30.4463 YY= -3.2283 ZY= 23.0859  
 XZ= -53.6703 YZ= 24.2450 ZZ= 129.5427  
 Eigenvalues: -24.8021 60.6456 166.3768

36 C Isotropic = 64.3333 Anisotropy = 143.1936  
 XX= 34.7933 YX= 33.1612 ZX= -49.8184  
 XY= 39.3368 YY= 82.2835 ZY= -47.8571  
 XZ= -36.2647 YZ= -63.2172 ZZ= 75.9232  
 Eigenvalues: 7.6180 25.5863 159.7957

37 C Isotropic = 71.8584 Anisotropy = 145.0453  
 XX= 76.1116 YX= 30.7121 ZX= -31.7343  
 XY= 19.7826 YY= 74.7127 ZY= -80.2603  
 XZ= -14.2162 YZ= -91.8956 ZZ= 64.7507  
 Eigenvalues: -16.4947 63.5146 168.5552

38 C Isotropic = 71.5704 Anisotropy = 144.2245  
 XX= 53.0051 YX= 71.4909 ZX= -2.4659  
 XY= 65.7741 YY= 72.8650 ZY= -50.6475  
 XZ= -20.2439 YZ= -65.1129 ZZ= 88.8412  
 Eigenvalues: -16.2312 63.2224 167.7201

39 C Isotropic = 64.6528 Anisotropy = 144.3537  
 XX= 39.0643 YX= 46.3469 ZX= -38.0619  
 XY= 29.5538 YY= 82.6275 ZY= -54.7627  
 XZ= -51.9736 YZ= -55.5039 ZZ= 72.2666  
 Eigenvalues: 7.6787 25.3911 160.8886

40 C Isotropic = 44.4555 Anisotropy = 79.7843  
 XX= 50.4220 YX= 18.0416 ZX= -12.6421  
 XY= 10.6573 YY= 43.9151 ZY= -47.9645  
 XZ= -26.8151 YZ= -39.7840 ZZ= 39.0292  
 Eigenvalues: -2.8973 38.6187 97.6450

41 C Isotropic = 44.3463 Anisotropy = 80.2940  
 XX= 27.7960 YX= 30.1041 ZX= -16.4148  
 XY= 39.6841 YY= 43.3953 ZY= -29.3233  
 XZ= -1.6873 YZ= -33.5931 ZZ= 61.8477  
 Eigenvalues: -3.1705 38.3338 97.8757

42 C Isotropic = 61.7372 Anisotropy = 163.0712  
 XX= 34.1694 YX= -6.0957 ZX= -88.1874  
 XY= 2.1716 YY= 36.7512 ZY= 1.1190  
 XZ= -86.4272 YZ= 7.4078 ZZ= 114.2911  
 Eigenvalues: -21.8366 36.5968 170.4514



43 C Isotropic = 67.9555 Anisotropy = 151.1209  
 XX= 81.0311 YX= -38.0926 ZX= -50.9090  
 XY= -28.8600 YY= -6.4001 ZY= -10.7003  
 XZ= -64.8681 YZ= -5.0856 ZZ= 129.2354  
 Eigenvalues: -23.0262 58.1899 168.7027

44 C Isotropic = 67.1610 Anisotropy = 148.8744  
 XX= 73.4555 YX= 23.6137 ZX= -55.7572  
 XY= 29.2825 YY= -8.6158 ZY= 20.7587  
 XZ= -48.5845 YZ= 26.9851 ZZ= 136.6431  
 Eigenvalues: -26.1452 61.2175 166.4105

45 C Isotropic = 53.3463 Anisotropy = 186.0115  
 XX= 26.6220 YX= 3.1898 ZX= -92.6440  
 XY= 0.4048 YY= 12.5706 ZY= 1.4553  
 XZ= -91.9359 YZ= 0.1636 ZZ= 120.8464  
 Eigenvalues: -29.9752 12.6601 177.3540

46 C Isotropic = 67.5578 Anisotropy = 148.3436  
 XX= 67.7989 YX= -31.7722 ZX= -58.2232  
 XY= -34.7710 YY= -0.9071 ZY= -18.2929  
 XZ= -51.7921 YZ= -19.5189 ZZ= 135.7816  
 Eigenvalues: -24.6218 60.8417 166.4535

47 C Isotropic = 65.9310 Anisotropy = 159.4501  
 XX= 76.5256 YX= 18.1005 ZX= -59.9071  
 XY= 23.8390 YY= -12.0492 ZY= 16.4500  
 XZ= -62.0297 YZ= 17.6119 ZZ= 133.3166  
 Eigenvalues: -23.8132 49.3752 172.2311

48 H Isotropic = 25.0485 Anisotropy = 8.1190  
 XX= 27.0943 YX= 2.9889 ZX= 3.4765  
 XY= 2.0152 YY= 25.1821 ZY= 0.9599  
 XZ= 3.6241 YZ= 1.0188 ZZ= 22.8692  
 Eigenvalues: 20.8101 23.8743 30.4612

49 H Isotropic = 25.0298 Anisotropy = 8.2411  
 XX= 27.2833 YX= -3.2372 ZX= 3.4968  
 XY= -2.1953 YY= 24.9778 ZY= -0.6066  
 XZ= 3.6444 YZ= -0.4209 ZZ= 22.8281  
 Eigenvalues: 20.6345 23.9309 30.5238

50 H Isotropic = 24.5324 Anisotropy = 9.9828  
 XX= 25.0278 YX= -1.4636 ZX= 5.1123  
 XY= -2.4552 YY= 24.0582 ZY= -1.0584  
 XZ= 6.2335 YZ= -1.4797 ZZ= 24.5113  
 Eigenvalues: 19.0489 23.3607 31.1876

51 H Isotropic = 24.9253 Anisotropy = 9.0931  
 XX= 28.0832 YX= 2.3191 ZX= 4.7340  
 XY= 2.0755 YY= 25.2692 ZY= 2.3157  
 XZ= 2.9799 YZ= 0.3362 ZZ= 21.4234  
 Eigenvalues: 19.6408 24.1477 30.9873

52 H Isotropic = 25.1257 Anisotropy = 8.7563  
 XX= 29.8651 YX= -3.0283 ZX= 3.6509  
 XY= -1.3490 YY= 23.7181 ZY= 1.1969  
 XZ= 1.3187 YZ= 2.3126 ZZ= 21.7939  
 Eigenvalues: 19.7053 24.7086 30.9632

53 H Isotropic = 25.0989 Anisotropy = 8.5637  
 XX= 25.2757 YX= -1.0305 ZX= 3.4517  
 XY= -0.6629 YY= 23.5764 ZY= 1.6119  
 XZ= 5.8043 YZ= 3.5427 ZZ= 26.4445  
 Eigenvalues: 19.7120 24.7767 30.8080

54 F Isotropic = 331.5053 Anisotropy = 161.9716  
 XX= 292.1822 YX= 27.7591 ZX= -63.1274  
 XY= 56.3206 YY= 327.5696 ZY= -61.7208  
 XZ= -34.9719 YZ= -49.3509 ZZ= 374.7642  
 Eigenvalues: 262.3794 292.6502 439.4864

55 F Isotropic = 331.7912 Anisotropy = 163.5584  
 XX= 326.7501 YX= 34.9982 ZX= -51.2224  
 XY= 35.6332 YY= 328.1492 ZY= -76.1692  
 XZ= -78.8594 YZ= -44.0356 ZZ= 340.4745  
 Eigenvalues: 262.1145 292.4290 440.8302

56 H Isotropic = 24.9365 Anisotropy = 8.9079  
 XX= 25.7212 YX= -1.3054 ZX= 3.8359  
 XY= -3.0244 YY= 25.4542 ZY= -1.0799  
 XZ= 5.5914 YZ= -2.2316 ZZ= 23.6341  
 Eigenvalues: 19.8490 24.0854 30.8751

57 H Isotropic = 24.5190 Anisotropy = 10.1632  
 XX= 29.3140 YX= 1.7482 ZX= 4.3334  
 XY= 1.7513 YY= 23.9381 ZY= 1.8261  
 XZ= 3.2631 YZ= 0.7416 ZZ= 20.3049  
 Eigenvalues: 18.8398 23.4227 31.2945

58 H Isotropic = 25.0400 Anisotropy = 8.1471  
 XX= 27.4095 YX= -3.2753 ZX= 3.2429  
 XY= -2.3520 YY= 25.3609 ZY= -0.6299  
 XZ= 3.0592 YZ= -0.5986 ZZ= 22.3497  
 Eigenvalues: 20.7193 23.9293 30.4714

59 H Isotropic = 24.9958 Anisotropy = 8.0075  
 XX= 27.6640 YX= 2.4144 ZX= 3.4869  
 XY= 1.8275 YY= 24.8157 ZY= 0.8848  
 XZ= 3.2320 YZ= 1.2077 ZZ= 22.5077  
 Eigenvalues: 20.8511 23.8022 30.3341

60 C Isotropic = 150.2546 Anisotropy = 32.9614  
 XX= 167.9117 YX= -1.2046 ZX= 18.8913  
 XY= -0.8998 YY= 138.8756 ZY= -0.6776  
 XZ= 3.0717 YZ= -0.4675 ZZ= 143.9765  
 Eigenvalues: 138.8075 139.7274 172.2289

61 C Isotropic = 152.0602 Anisotropy = 41.0476  
 XX= 179.3778 YX= -1.5047 ZX= 4.3558  
 XY= -1.3041 YY= 133.7865 ZY= -0.3340  
 XZ= -3.5809 YZ= -0.1441 ZZ= 143.0164  
 Eigenvalues: 133.7377 143.0177 179.4253

62 C Isotropic = 154.7038 Anisotropy = 33.1716  
 XX= 176.7669 YX= -1.1640 ZX= -0.4563  
 XY= -1.1369 YY= 137.4047 ZY= -0.1047  
 XZ= -0.9286 YZ= -0.1589 ZZ= 149.9397  
 Eigenvalues: 137.3693 149.9239 176.8181

63 C Isotropic = 163.5732 Anisotropy = 20.9564  
 XX= 176.6763 YX= -0.7457 ZX= 0.1290  
 XY= -0.5978 YY= 151.6126 ZY= -0.2417  
 XZ= -7.3050 YZ= 0.0057 ZZ= 162.4306  
 Eigenvalues: 151.5902 161.5852 177.5441

64 C Isotropic = 173.7273 Anisotropy = 23.9833  
 XX= 187.0118 YX= -0.7731 ZX= 4.2866  
 XY= -0.9637 YY= 163.6659 ZY= -0.2022  
 XZ= 10.0297 YZ= -0.4267 ZZ= 170.5042  
 Eigenvalues: 163.6331 167.8326 189.7161

65 H Isotropic = 29.6328 Anisotropy = 4.5058  
 XX= 30.0891 YX= -0.8520 ZX= 0.7841  
 XY= -2.0296 YY= 29.4003 ZY= 2.5253  
 XZ= 2.0524 YZ= 3.9384 ZZ= 29.4089  
 Eigenvalues: 25.3164 30.9453 32.6366

66 H Isotropic = 29.6843 Anisotropy = 4.4078  
 XX= 30.2788 YX= 0.7009 ZX= 0.5930  
 XY= 1.7782 YY= 29.6148 ZY= -2.4444  
 XZ= 1.8405 YZ= -4.0047 ZZ= 29.1592  
 Eigenvalues: 25.5214 30.9086 32.6228

67 H Isotropic = 30.5344 Anisotropy = 4.7927  
 XX= 33.5727 YX= 0.3970 ZX= 1.1881  
 XY= 0.5653 YY= 29.2224 ZY= 3.1197  
 XZ= -1.0958 YZ= 4.3117 ZZ= 28.8082  
 Eigenvalues: 25.2832 32.5906 33.7296

68 H Isotropic = 30.5290 Anisotropy = 4.8840  
 XX= 33.5434 YX= -0.7932 ZX= 1.0051  
 XY= -0.8008 YY= 29.6120 ZY= -2.9425  
 XZ= -1.4149 YZ= -4.0659 ZZ= 28.4317  
 Eigenvalues: 25.4127 32.3893 33.7850

69 H Isotropic = 30.7159 Anisotropy = 4.3164  
 XX= 32.4747 YX= 0.2870 ZX= 0.6747  
 XY= 0.0036 YY= 30.0257 ZY= 3.0540  
 XZ= 0.4256 YZ= 4.0266 ZZ= 29.6472  
 Eigenvalues: 26.2766 32.2775 33.5934

70 H Isotropic = 30.7261 Anisotropy = 4.2724  
 XX= 32.4400 YX= -0.5117 ZX= 0.4631  
 XY= -0.1648 YY= 30.3846 ZY= -2.9799  
 XZ= 0.1948 YZ= -3.9634 ZZ= 29.3536  
 Eigenvalues: 26.3592 32.2446 33.5743

71 H Isotropic = 30.6699 Anisotropy = 6.0327  
 XX= 31.8017 YX= -0.4601 ZX= 0.1877  
 XY= -0.6488 YY= 29.6075 ZY= 4.2560  
 XZ= -0.1073 YZ= 4.7844 ZZ= 30.6004  
 Eigenvalues: 25.5257 31.7922 34.6917

72 H Isotropic = 30.6630 Anisotropy = 5.9004  
 XX= 31.8646 YX= 0.2918 ZX= -0.0181  
 XY= 0.5579 YY= 29.9291 ZY= -4.1961  
 XZ= -0.3571 YZ= -4.7328 ZZ= 30.1954  
 Eigenvalues: 25.5910 31.8015 34.5966

73 H Isotropic = 31.0316 Anisotropy = 10.0814  
 XX= 36.8523 YX= -0.2332 ZX= -3.2793  
 XY= -0.2400 YY= 26.8507 ZY= 0.0610  
 XZ= -2.1900 YZ= 0.0239 ZZ= 29.3919  
 Eigenvalues: 26.8448 28.4976 37.7526

74 H Isotropic = 31.2252 Anisotropy = 7.9507  
 XX= 31.6599 YX= 2.2490 ZX= 2.9321  
 XY= 1.6469 YY= 31.7748 ZY= 3.1329  
 XZ= 1.9619 YZ= 3.8680 ZZ= 30.2409  
 Eigenvalues: 27.2735 29.8763 36.5257

75 H Isotropic = 31.2355 Anisotropy = 7.9188  
 XX= 31.4393 YX= -2.3701 ZX= 2.6491  
 XY= -1.6663 YY= 32.2924 ZY= -3.1767  
 XZ= 1.6782 YZ= -3.8686 ZZ= 29.9748  
 Eigenvalues: 27.3172 29.8746 36.5147

76 C Isotropic = 67.5887 Anisotropy = 147.1135  
 XX= 77.5974 YX= -21.5415 ZX= 61.0938  
 XY= -24.8370 YY= 0.4153 ZY= 33.7530  
 XZ= 55.5846 YZ= 34.9392 ZZ= 124.7533  
 Eigenvalues: -24.4242 61.5258 165.6644

77 C Isotropic = 66.0902 Anisotropy = 159.2298  
 XX= 79.4172 YX= 27.4997 ZX= 61.2979  
 XY= 33.7456 YY= -10.3684 ZY= -3.2529  
 XZ= 62.7112 YZ= -4.3783 ZZ= 129.2217  
 Eigenvalues: -23.7294 49.7566 172.2434

78 C Isotropic = 62.0581 Anisotropy = 162.5785  
 XX= 42.1812 YX= 1.5323 ZX= 90.7987  
 XY= 9.4993 YY= 37.6429 ZY= 9.5223  
 XZ= 89.3689 YZ= 3.6356 ZZ= 106.3502  
 Eigenvalues: -21.3700 37.1005 170.4438

79 C Isotropic = 67.9516 Anisotropy = 150.8792  
 XX= 90.0672 YX= -28.2754 ZX= 54.4160  
 XY= -17.1223 YY= -7.5153 ZY= 25.4442  
 XZ= 67.1457 YZ= 19.9972 ZZ= 121.3030  
 Eigenvalues: -22.9981 58.3152 168.5378

80 C Isotropic = 67.0351 Anisotropy = 150.0071  
 XX= 75.2061 YX= 31.6528 ZX= 58.1794  
 XY= 37.5836 YY= -8.1428 ZY= -7.6760  
 XZ= 50.9460 YZ= -14.0718 ZZ= 134.0420  
 Eigenvalues: -26.5245 60.5900 167.0399

81 C Isotropic = 64.7948 Anisotropy = 143.4781  
 XX= 37.8892 YX= 47.9129 ZX= 31.6434  
 XY= 32.8625 YY= 96.1670 ZY= 53.1034  
 XZ= 47.4532 YZ= 54.2868 ZZ= 60.3281  
 Eigenvalues: 7.9989 25.9385 160.4468

82 C Isotropic = 44.7055 Anisotropy = 80.5371  
 XX= 49.6712 YX= 20.5800 ZX= 7.3823  
 XY= 14.7344 YY= 53.6412 ZY= 46.7550  
 XZ= 22.9136 YZ= 40.4912 ZZ= 30.8041  
 Eigenvalues: -2.9011 38.6207 98.3969

83 C Isotropic = 44.7054 Anisotropy = 80.3700  
 XX= 23.9140 YX= 30.9357 ZX= 13.2794  
 XY= 38.8285 YY= 53.1403 ZY= 30.1200  
 XZ= -2.3157 YZ= 33.2932 ZZ= 57.0617  
 Eigenvalues: -2.7502 38.5809 98.2853

84 C Isotropic = 64.6081 Anisotropy = 144.5174  
 XX= 32.2001 YX= 35.2238 ZX= 45.4497  
 XY= 39.4245 YY= 96.2965 ZY= 48.9151  
 XZ= 29.9890 YZ= 64.1714 ZZ= 65.3278  
 Eigenvalues: 7.5645 25.3068 160.9531

85 C Isotropic = 71.7995 Anisotropy = 143.8216  
 XX= 74.2183 YX= 34.3768 ZX= 23.7857  
 XY= 22.8815 YY= 90.3764 ZY= 79.4944  
 XZ= 6.6051 YZ= 88.2928 ZZ= 50.8039  
 Eigenvalues: -16.0115 63.7296 167.6806

86 C Isotropic = 72.0562 Anisotropy = 144.2124  
 XX= 45.2308 YX= 71.1515 ZX= -4.6403  
 XY= 66.7545 YY= 90.2482 ZY= 49.5138  
 XZ= 12.3214 YZ= 63.3630 ZZ= 80.6895  
 Eigenvalues: -15.8228 63.7935 168.1978

87 C Isotropic = 61.8095 Anisotropy = 162.7187  
 XX= 39.0775 YX= 3.8279 ZX= 88.4370  
 XY= 6.6835 YY= 37.4529 ZY= 12.2345  
 XZ= 89.7405 YZ= 2.5002 ZZ= 108.8982  
 Eigenvalues: -21.6973 36.8373 170.2887

88 C Isotropic = 66.1456 Anisotropy = 159.1373  
 XX= 82.1252 YX= -13.6173 ZX= 64.0729  
 XY= -14.8021 YY= -9.5958 ZY= 31.1665  
 XZ= 62.5920 YZ= 24.9493 ZZ= 125.9073  
 Eigenvalues: -23.5116 49.7113 172.2371

89 C Isotropic = 67.5182 Anisotropy = 147.8277  
 XX= 81.0396 YX= 39.8033 ZX= 56.8980  
 XY= 40.3198 YY= -0.4477 ZY= -10.7196  
 XZ= 62.1281 YZ= -7.2902 ZZ= 121.9627  
 Eigenvalues: -24.4974 60.9819 166.0700

90 C Isotropic = 53.4012 Anisotropy = 185.5767  
 XX= 38.0401 YX= 8.7949 ZX= 95.6705  
 XY= 8.8927 YY= 14.7289 ZY= 12.7706  
 XZ= 97.5454 YZ= 15.7924 ZZ= 107.4347  
 Eigenvalues: -29.9348 13.0195 177.1190

91 C Isotropic = 67.0506 Anisotropy = 148.7746  
 XX= 90.7502 YX= -24.2418 ZX= 56.7736  
 XY= -20.4625 YY= -7.0190 ZY= 32.9087  
 XZ= 63.6293 YZ= 25.8338 ZZ= 117.4205  
 Eigenvalues: -26.1425 61.0606 166.2336

92 C Isotropic = 67.6792 Anisotropy = 150.8942  
 XX= 77.4012 YX= 29.0667 ZX= 62.3072  
 XY= 29.8477 YY= -8.1404 ZY= -6.3198  
 XZ= 49.3365 YZ= -18.0724 ZZ= 133.7767  
 Eigenvalues: -23.2252 57.9874 168.2753

93 H Isotropic = 25.0566 Anisotropy = 8.2227  
 XX= 27.5181 YX= -3.3536 ZX= -3.2591  
 XY= -2.4599 YY= 25.1715 ZY= 0.2631  
 XZ= -3.1769 YZ= 0.4409 ZZ= 22.4801  
 Eigenvalues: 20.6585 23.9728 30.5384

94 H Isotropic = 25.0168 Anisotropy = 8.2183  
 XX= 27.3187 YX= 2.4255 ZX= -3.8089  
 XY= 1.6970 YY= 24.8220 ZY= -1.3022  
 XZ= -3.5318 YZ= -1.5532 ZZ= 22.9098  
 Eigenvalues: 20.8170 23.7378 30.4957

95 H Isotropic = 24.5176 Anisotropy = 10.1504  
 XX= 28.8089 YX= 1.4978 ZX= -4.6794  
 XY= 1.6684 YY= 23.8595 ZY= -2.4565  
 XZ= -3.6754 YZ= -1.4724 ZZ= 20.8845  
 Eigenvalues: 18.7897 23.4786 31.2846

96 H Isotropic = 24.9400 Anisotropy = 8.9636  
 XX= 25.6532 YX= -1.4988 ZX= -3.9007  
 XY= -3.4211 YY= 25.3922 ZY= 0.8336  
 XZ= -5.6204 YZ= 1.7580 ZZ= 23.7746  
 Eigenvalues: 19.7965 24.1077 30.9157

97 H Isotropic = 25.1025 Anisotropy = 8.6292  
 XX= 25.1060 YX= -1.3037 ZX= -3.2684  
 XY= -1.0081 YY= 23.0775 ZY= -1.5095  
 XZ= -5.5311 YZ= -3.5759 ZZ= 27.1241  
 Eigenvalues: 19.6901 24.7621 30.8553

98 H Isotropic = 25.0681 Anisotropy = 8.7119  
 XX= 29.8140 YX= -2.9952 ZX= -3.6483  
 XY= -1.1012 YY= 23.0137 ZY= -1.4468  
 XZ= -1.4992 YZ= -2.5311 ZZ= 22.3765  
 Eigenvalues: 19.6204 24.7078 30.8760

99 F Isotropic = 332.3378 Anisotropy = 164.2304  
 XX= 326.3315 YX= 39.6313 ZX= 43.8259  
 XY= 43.3783 YY= 342.3864 ZY= 77.9943  
 XZ= 74.2712 YZ= 47.4230 ZZ= 328.2954  
 Eigenvalues: 262.4975 292.6911 441.8247

100 F Isotropic = 332.7810 Anisotropy = 165.8689  
 XX= 289.8354 YX= 31.6570 ZX= 60.9061  
 XY= 58.7359 YY= 343.4184 ZY= 68.5567  
 XZ= 30.2932 YZ= 54.3645 ZZ= 365.0891  
 Eigenvalues: 262.3497 292.6330 443.3603

101 H Isotropic = 24.5282 Anisotropy = 10.0870  
 XX= 24.6822 YX= -1.9796 ZX= -5.1610  
 XY= -2.9384 YY= 23.9412 ZY= 0.7742  
 XZ= -6.2079 YZ= 0.8976 ZZ= 24.9613  
 Eigenvalues: 18.8377 23.4941 31.2529

102 H Isotropic = 24.9427 Anisotropy = 8.9651  
 XX= 27.2451 YX= 2.1841 ZX= -4.9567  
 XY= 1.9833 YY= 25.3607 ZY= -2.9051  
 XZ= -3.3032 YZ= -0.8367 ZZ= 22.2223  
 Eigenvalues: 19.8222 24.0864 30.9194

103 H Isotropic = 25.0340 Anisotropy = 7.9579  
 XX= 25.9937 YX= -2.3193 ZX= -3.8780  
 XY= -1.8033 YY= 24.9837 ZY= 1.0802  
 XZ= -4.2322 YZ= 1.5966 ZZ= 24.1245  
 Eigenvalues: 20.8812 23.8815 30.3392

104 H Isotropic = 25.0367 Anisotropy = 8.0817  
 XX= 25.3364 YX= 1.5922 ZX= -3.9676  
 XY= 1.0430 YY= 25.1123 ZY= -2.1531  
 XZ= -4.1141 YZ= -2.8804 ZZ= 24.6614  
 Eigenvalues: 20.6859 23.9996 30.4245

105 C Isotropic = 150.6683 Anisotropy = 32.5653  
 XX= 155.5791 YX= 0.6398 ZX= -7.5744  
 XY= -0.3338 YY= 139.4202 ZY= 0.3446  
 XZ= -24.5642 YZ= -0.5676 ZZ= 157.0056  
 Eigenvalues: 139.4177 140.2087 172.3785

106 C Isotropic = 151.6105 Anisotropy = 40.6051  
 XX= 149.7142 YX= 0.4190 ZX= -10.4679  
 XY= -0.0426 YY= 133.0891 ZY= 1.6324  
 XZ= -17.2180 YZ= 1.1393 ZZ= 172.0283  
 Eigenvalues: 133.0008 143.1502 178.6806

107 C Isotropic = 155.3132 Anisotropy = 33.1831  
 XX= 153.8855 YX= 0.4748 ZX= -8.1844  
 XY= 0.3641 YY= 138.0271 ZY= 1.7358  
 XZ= -9.5804 YZ= 1.6040 ZZ= 174.0271  
 Eigenvalues: 137.9000 150.6043 177.4353

108 C Isotropic = 162.9373 Anisotropy = 20.5544  
 XX= 162.5120 YX= 0.7767 ZX= -0.0919  
 XY= 0.2921 YY= 150.4268 ZY= 1.6234  
 XZ= -6.2027 YZ= 1.2448 ZZ= 175.8731  
 Eigenvalues: 150.3036 161.8681 176.6403

109 C Isotropic = 173.6810 Anisotropy = 24.0435  
 XX= 178.7201 YX= 0.1719 ZX= -13.5228  
 XY= 0.3960 YY= 163.0105 ZY= 0.2307  
 XZ= -7.8560 YZ= 0.5236 ZZ= 179.3125  
 Eigenvalues: 162.9696 168.3634 189.7100

110 H Isotropic = 29.5585 Anisotropy = 4.6938  
 XX= 30.6521 YX= -3.3270 ZX= -1.4669  
 XY= -1.8169 YY= 28.6220 ZY= -3.1519  
 XZ= -0.5041 YZ= -2.3666 ZZ= 29.4015  
 Eigenvalues: 25.0099 30.9780 32.6877

111 H Isotropic = 29.6119 Anisotropy = 4.5496  
 XX= 30.0199 YX= 3.1355 ZX= -2.2558  
 XY= 1.8157 YY= 30.0668 ZY= 2.6359  
 XZ= -0.9181 YZ= 2.0486 ZZ= 28.7490  
 Eigenvalues: 25.3038 30.8869 32.6450

112 H Isotropic = 30.4868 Anisotropy = 4.7851  
 XX= 29.8929 YX= -4.1371 ZX= -0.3898  
 XY= -3.0702 YY= 28.8626 ZY= -0.2582  
 XZ= -2.6221 YZ= -1.1748 ZZ= 32.7050  
 Eigenvalues: 25.4146 32.3690 33.6769

113 H Isotropic = 30.4647 Anisotropy = 4.8133  
XX= 28.9087 YX= 3.9477 ZX= -0.9624  
XY= 2.4656 YY= 29.9637 ZY= 0.5029  
XZ= -3.1957 YZ= 1.0629 ZZ= 32.5217  
Eigenvalues: 25.5516 32.1689 33.6736

114 H Isotropic = 30.6894 Anisotropy = 4.5510  
XX= 30.7653 YX= -3.8996 ZX= -0.8791  
XY= -3.2277 YY= 29.4284 ZY= -1.3659  
XZ= -1.2647 YZ= -1.3200 ZZ= 31.8745  
Eigenvalues: 25.9712 32.3737 33.7234

115 H Isotropic = 30.7103 Anisotropy = 4.4762  
XX= 29.8586 YX= 3.7239 ZX= -1.5297  
XY= 3.0019 YY= 30.7227 ZY= 1.3357  
XZ= -1.8071 YZ= 1.2252 ZZ= 31.5495  
Eigenvalues: 26.0927 32.3436 33.6944

116 H Isotropic = 30.6944 Anisotropy = 5.7782  
XX= 31.2194 YX= -4.1232 ZX= 0.0770  
XY= -3.2534 YY= 29.0017 ZY= -1.8643  
XZ= -0.1361 YZ= -2.1552 ZZ= 31.8622  
Eigenvalues: 25.8075 31.7292 34.5466

117 H Isotropic = 30.6739 Anisotropy = 5.6687  
XX= 30.2017 YX= 4.1820 ZX= -0.7478  
XY= 3.2152 YY= 30.5213 ZY= 2.0358  
XZ= -0.8779 YZ= 2.3054 ZZ= 31.2989  
Eigenvalues: 25.8418 31.7270 34.4531

118 H Isotropic = 31.1071 Anisotropy = 10.0075  
XX= 28.7871 YX= 0.0376 ZX= -1.4492  
XY= 0.0948 YY= 26.8686 ZY= 0.5902  
XZ= -0.2161 YZ= 0.6764 ZZ= 37.6656  
Eigenvalues: 26.8247 28.7179 37.7788

119 H Isotropic = 31.2608 Anisotropy = 7.8959  
XX= 32.6931 YX= -4.5584 ZX= -1.2123  
XY= -3.7146 YY= 31.4337 ZY= -0.0407  
XZ= -2.2491 YZ= 0.2061 ZZ= 29.6556  
Eigenvalues: 27.3403 29.9174 36.5247

120 H Isotropic = 31.2701 Anisotropy = 7.8448  
XX= 31.6645 YX= 4.3795 ZX= -1.7476  
XY= 3.3877 YY= 32.3814 ZY= -0.4494  
XZ= -2.6154 YZ= -0.8417 ZZ= 29.7643  
Eigenvalues: 27.4009 29.9094 36.5000



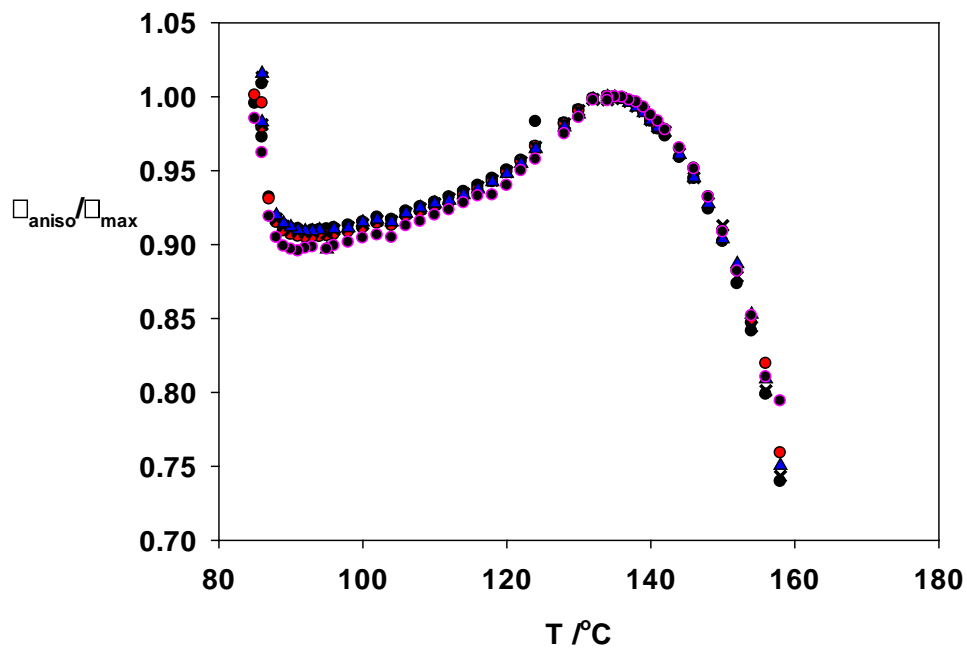


Figure S1. The chemical shift anisotropies,  $\delta_{\text{aniso}}$ , scaled by the maximum value reached in the nematic phase of DTC5C9 for the four well-resolved resonances of carbons on the *para* axis, C10, C16, C1 and C13.

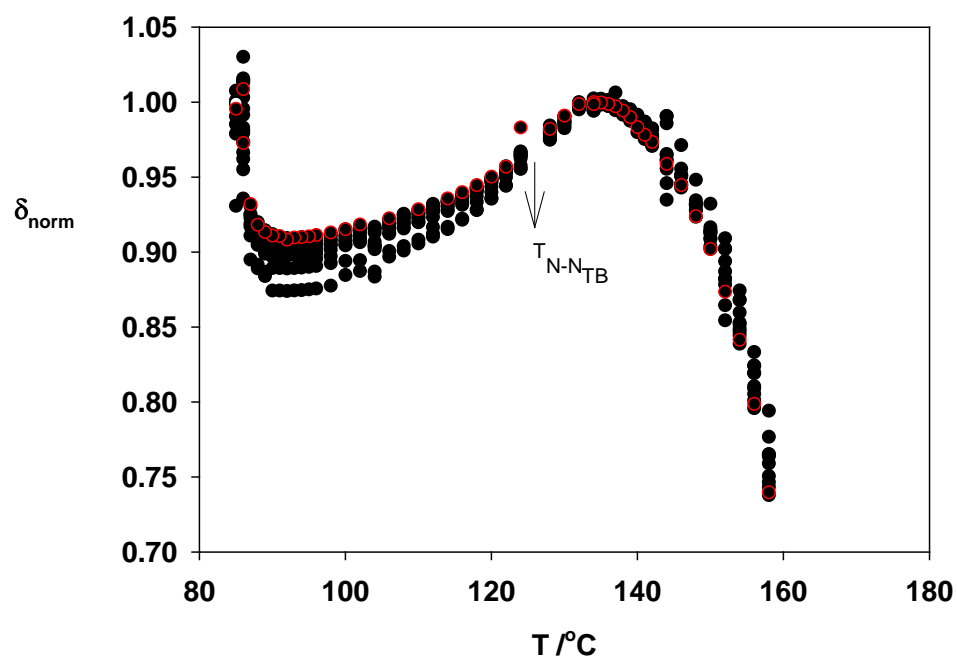


Figure S2. The chemical shift anisotropies,  $\delta_{\text{aniso}}$ , scaled by the maximum value,  $\delta_{\text{max}}$ , reached in the nematic phase of DTC5C9 for all the well-resolved resonances of the carbon nuclei in the difluoroterphenyl group.

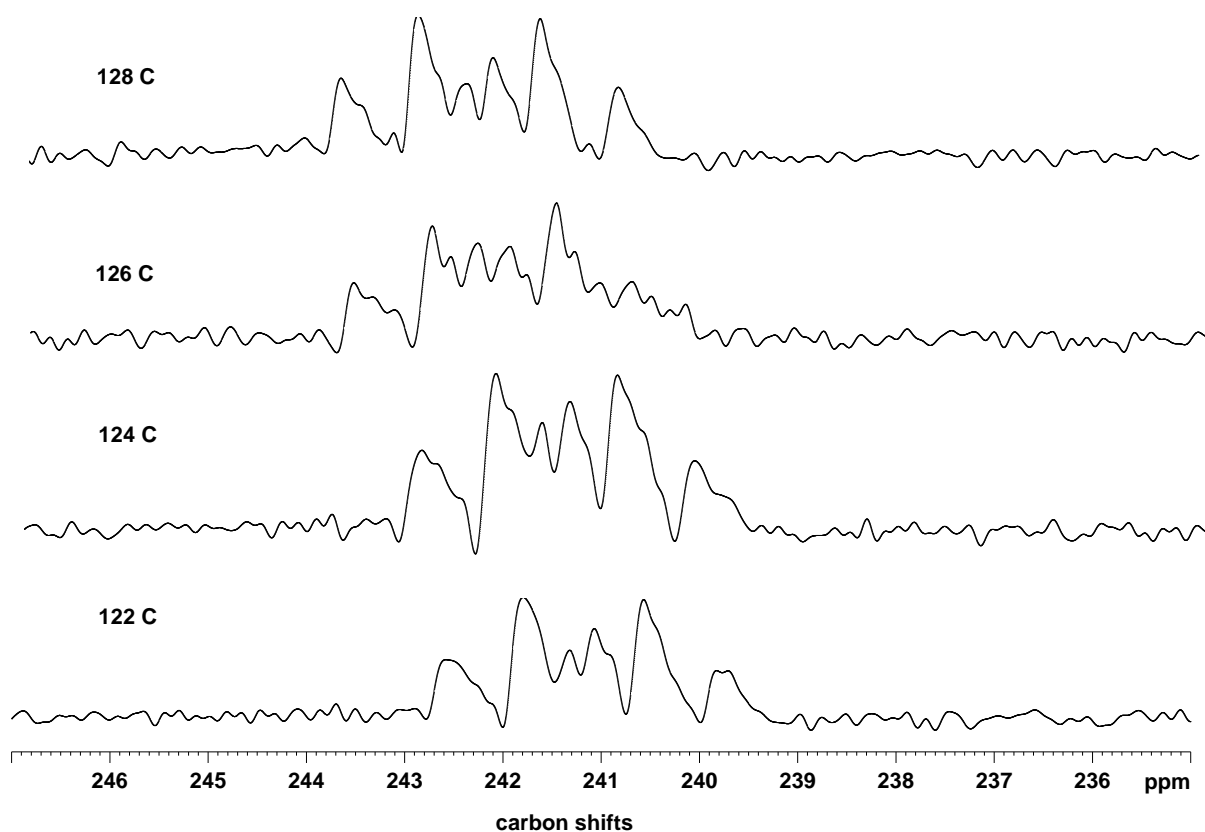


Fig. S3. The 125 MHz  $^{13}\text{C}$  -  $\{^1\text{H}\}$  spectra of C10 and C16 from just above to just below the transition from  $N_U$  to  $N_{TB}$ . At  $T = 128^\circ\text{C}$  the sample is wholly in the  $N_U$  phase, whilst both  $N_U$  and  $N_{TB}$  phases are present at  $126^\circ\text{C}$ . The sample is entirely in the  $N_{TB}$  phase at  $124^\circ\text{C}$  and  $122^\circ\text{C}$ .

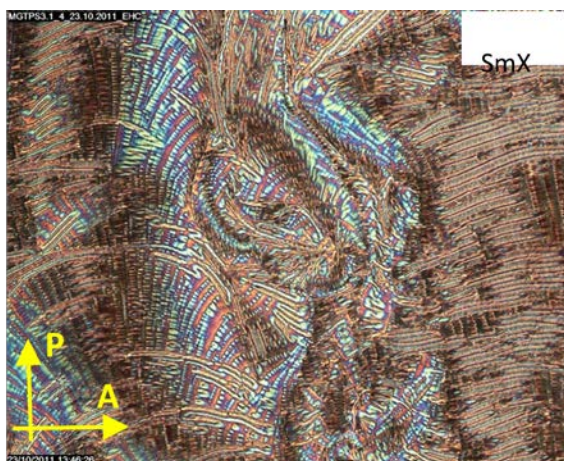


Figure S4. Polarising microscopy of DTC5C9 at 75 °C in the SmX phase: magnification x100, crossed polarizers, 6  $\mu\text{m}$  EHC cell, uncoated.

## References

1. GAUSSIAN 09 (Revision A.02), Gaussian Inc., Wallingford CT, U.S.A., **2009**.