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

J.W. Emsley[1*], M. Lelli[3], H. Joy[2], M.-G. Tamba[2], G.H. Mehl[2]

[1]Department of Chemistry, University of Southampton, Southampton SO17 1BJ, UK.

[2]Department of Chemistry, University of Hull, Hull HU6 7RX.

[3] Institut des Sciences Analytiques, Centre RMN à Très Hauts Champs (CRMN), CNRS/ENS Lyon/ UCB-Lyon 1, 5 rue de la Doua, 69100 Villeurbanne, France.

Table S1. The differences, Δ_i /ppm for ^{13}C nuclei in DTC5C9. The values of δ_i were taken from a spectrum recorded in the isotropic phase at 166 °C.

	Carbon site						
T / °C	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

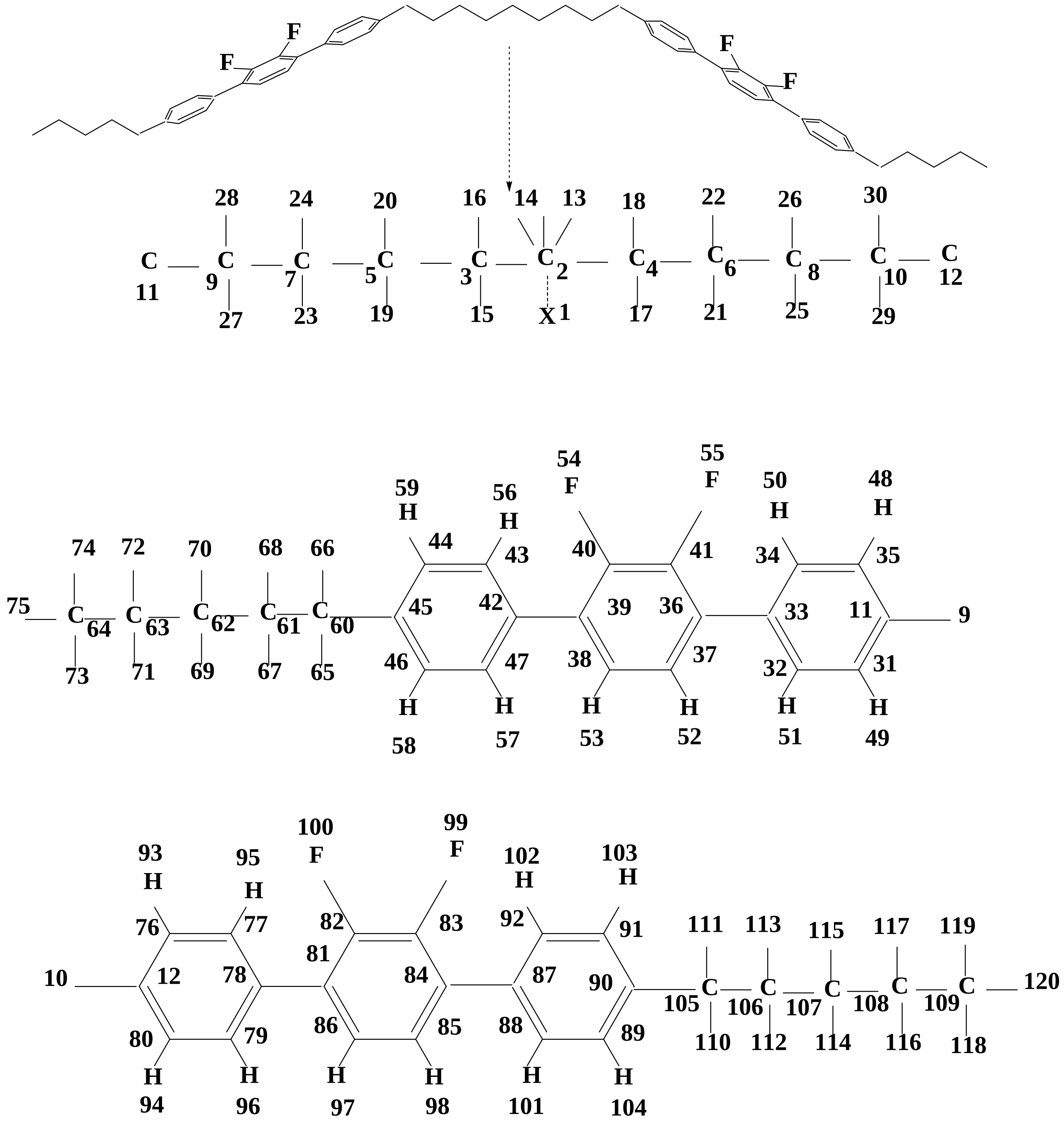
95	43.852	42.531	15.015	15.015	-1.674	-2.297
94	43.828	42.503	14.995	14.971	-1.667	-2.309
93	43.816	42.483	15.085	14.968	-1.662	-2.326
92	43.748	42.487	15.078	14.971	-1.657	-2.335
91	43.864	42.509	15.076	14.971	-1.655	-2.339
90	43.876	42.568	15.088	14.988	-1.653	-2.347
89	43.992	42.682	15.121	15.024	-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}C resonances in the ^{13}C – {^{1}H} spectra of Mehl compound.

	Average D_{CF} for each ring carbon/Hz											
T/ °C	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, θ_{ijk}, and dihedral angles, δ_{ijks}, of DTC5C9 in the most elongated conformation, calculated by the DFT method[1] B3LYP/6-31G*.

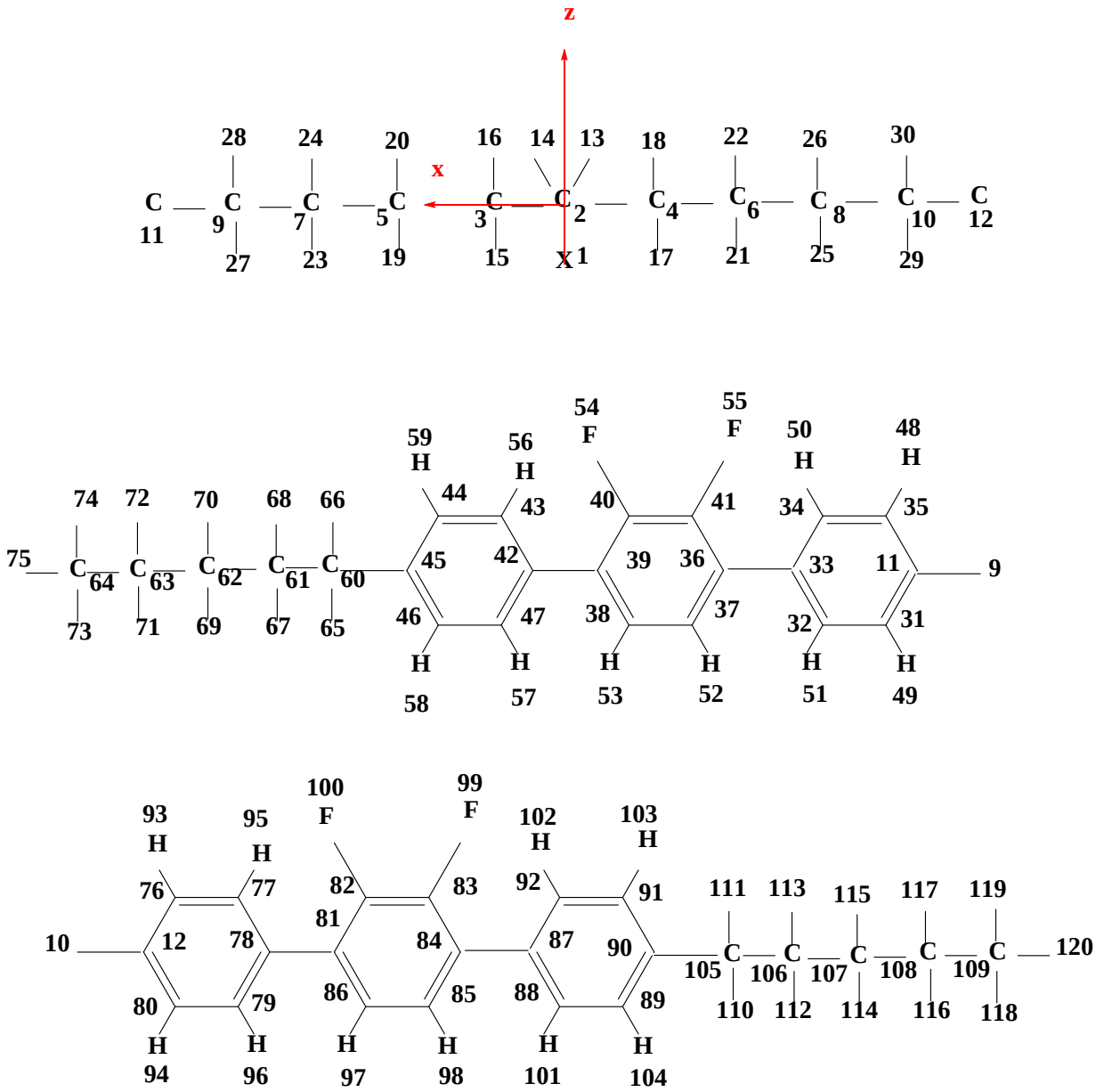


i		j	$r_{i,j}$ /Å	k	$\theta_{i,j,k}$ /°	s	$\delta_{I,j,k,s}$ /°
1	X						
2	C	1	1.000*				
3	C	2	1.534	1	123.2		
4	C	2	1.534	1	123.2	3	180.0*
5	C	3	1.534	2	113.3	4	180.0
6	C	4	1.534	2	113.3	3	180.5
7	C	5	1.534	3	113.6	2	179.8
8	C	6	1.534	4	113.6	2	181.1
9	C	7	1.543	5	113.0	3	179.9
10	C	8	1.543	6	113.0	4	180.9
11	C	9	1.513	7	113.2	5	179.5
12	C	10	1.513	8	113.2	6	181.0
13	H	2	1.100	3	109.2	4	122.3
14	H	2	1.100	3	109.2	4	-122.3
15	H	3	1.100	2	109.3	5	122.2
16	H	3	1.100	2	109.3	5	-122.2
17	H	4	1.100	2	109.3	6	122.2
18	H	4	1.100	2	109.3	6	-122.2
19	H	5	1.100	3	109.3	7	122.3
20	H	5	1.100	3	109.3	7	-122.2
21	H	6	1.100	4	109.3	8	122.2
22	H	6	1.100	4	109.3	8	-122.3
23	H	7	1.099	5	109.7	9	121.9
24	H	7	1.099	5	109.7	9	-122.0
25	H	8	1.099	6	109.7	10	121.9
26	H	8	1.099	6	109.7	10	-121.9
27	H	9	1.098	7	108.9	11	122.2
28	H	9	1.098	7	108.9	11	-122.1
29	H	10	1.098	8	108.9	12	122.1
30	H	10	1.098	8	108.9	12	-122.2
31	C	11	1.401	9	121.2	7	89.0
32	C	31	1.393	11	121.2	9	181.8
33	C	32	1.405	31	121.1	11	-0.1
34	C	33	1.405	32	117.8	31	0.4
35	C	34	1.392	33	120.8	32	-0.5
36	C	33	1.483	32	120.1	31	181.9
37	C	36	1.407	33	121.6	32	37.1
38	C	37	1.389	36	122.0	33	180.4
39	C	38	1.408	37	122.0	36	0.0
40	C	39	1.399	38	115.9	37	0.0
41	C	40	1.393	39	122.1	38	0.0
42	C	39	1.483	40	122.6	41	180.2
43	C	42	1.405	39	120.1	40	142.3
44	C	43	1.393	42	121.1	39	178.4
45	C	44	1.401	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
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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

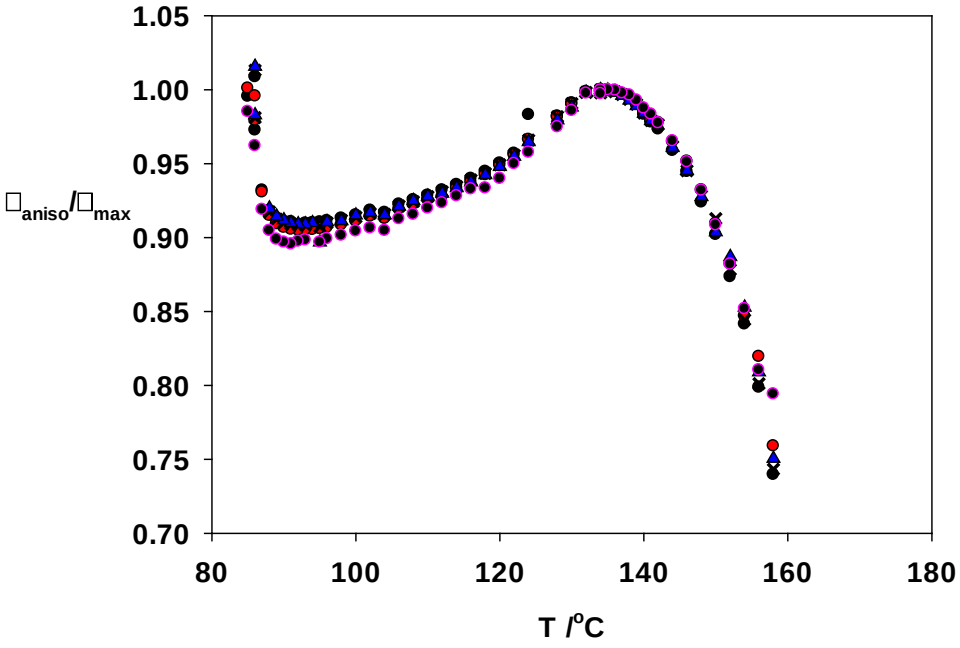

Figure S1. The chemical shift anisotropies, δ_{aniso}, scaled by the maximum value reached in the nematic phase of DTC5C9 for the four well-resolved resonances of carbons on the *para* axis , C10, C16, C1 and C13.

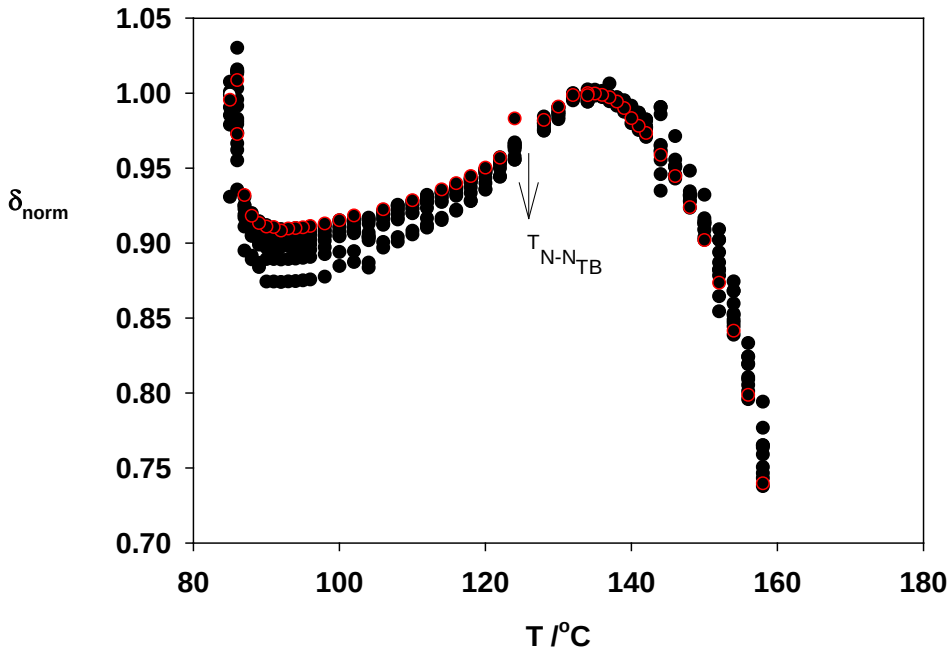

Figure S2. The chemical shift anisotropies, δ_{aniso}, scaled by the maximum value, δ_{max}, reached in the nematic phase of DTC5C9 for all the well-resolved resonances of the carbon nuclei in the difluoroterphenyl group.

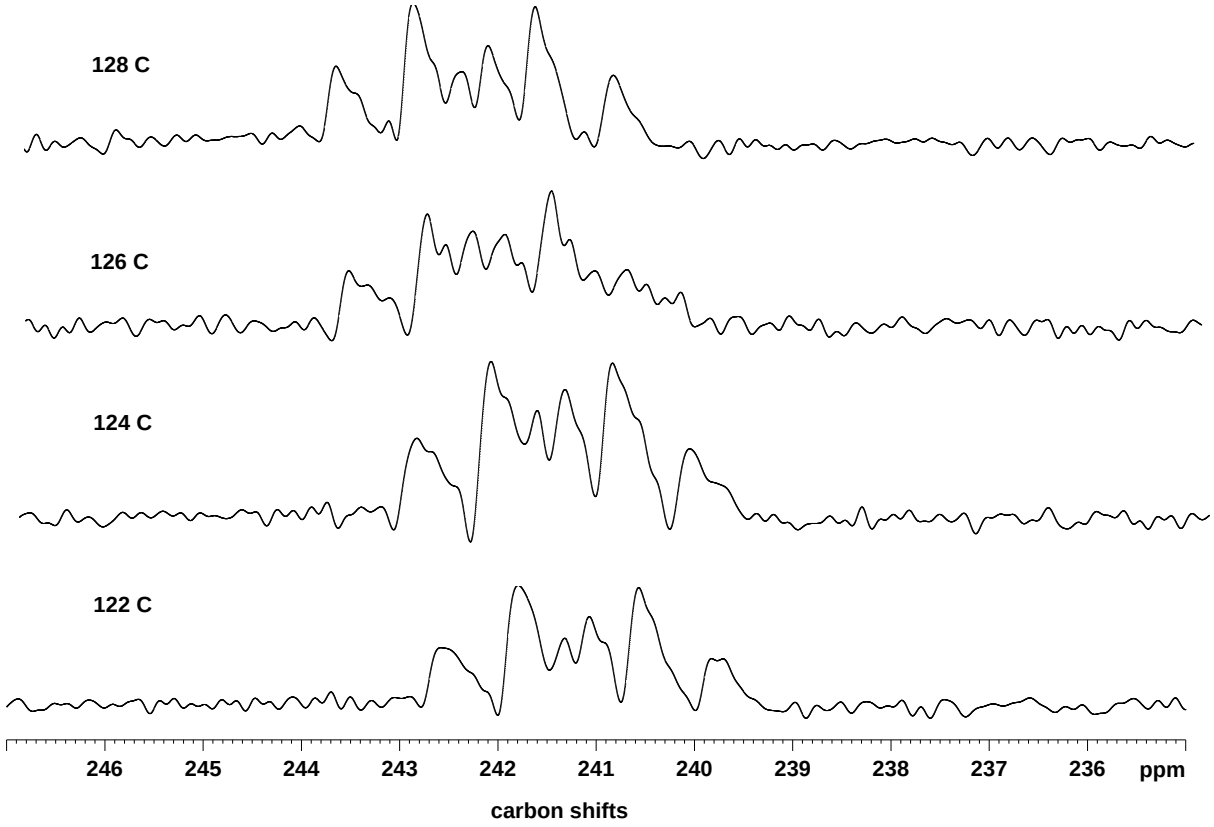

Fig. S3. The 125 MHz ^{13}C - $\{^1H\}$ spectra of C10 and C16 from just above to just below the transition from N_U to N_{TB}. At T = 128° C the sample is wholly in the N_U phase, whilst both N_U and N_{TB} phases are present at 126° C. The sample is entirely in the N_{TB} phase at 124° and 122° C.

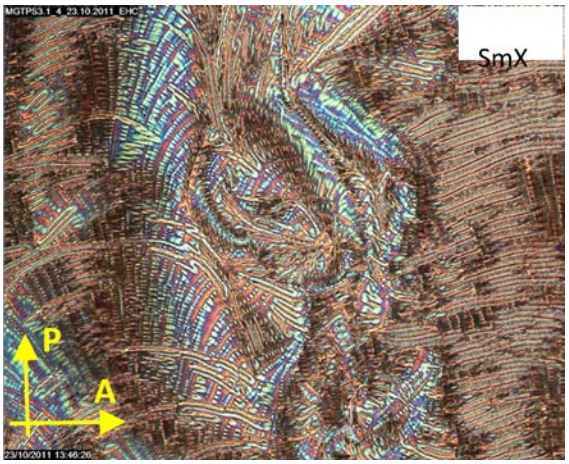

Figure S4. Polarising microscopy of DTC5C9 at 75 °C in the SmX phase: magnification x100, crossed polarizers, 6 µm EHC cell, uncoated.

References

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