Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Vibrational circular dichroism studies of exceptionally strong chirality inducers in liquid crystals

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NM	τ	Freq.	R_{01}	$R_{01}^{\mathbf{GCO}}$	$\lvert\vec{E}_{01}^{A}\rvert$	$\lvert\vec{E}_{01}^{B}\rvert$	$\lvert\vec{E}_{01}^{A} \times \vec{E}_{01}^{B}\rvert$	ξ
201	47.2	1069.2	329.0	229.6	10.6	13.9	86.55	35.9
201	57.0	1069.9	302.3	212.1	10.7	14.2	83.64	33.4
201	**68.5**	**1070.5**	**280.7**	**192.1**	**10.8**	**14.2**	**78.94**	**31.0**
201	78.5	1070.4	259.8	176.7	10.9	14.3	76.91	29.6
201	88.5	1070.0	246.6	164.1	11.0	14.4	75.47	28.5
209	47.2	1117.6	-67.9	-64.2	4.8	5.6	27.06	98.3
209	57.0	1118.5	-66.1	-61.8	4.7	5.8	26.88	101.5
209	**68.5**	**1119.2**	**-65.7**	**-61.6**	**4.8**	**6.0**	**27.42**	**104.7**
209	78.5	1119.5	-65.5	-61.6	4.9	6.2	28.87	107.5
209	88.5	1120.0	-67.2	-64.7	5.2	6.6	31.77	110.9
223	47.2	1187.6	-396.6	-365.7	11.8	20.7	205.27	122.9
223	57.0	1188.8	-403.5	-362.8	11.7	21.9	211.02	124.6
223	**68.5**	**1189.9**	**-383.7**	**-331.6**	**11.0**	**22.5**	**199.83**	**126.6**
223	78.5	1189.7	-377.2	-321.3	11.1	23.0	195.76	129.7
223	88.5	1189.2	-373.5	-312.9	11.3	23.1	191.87	132.4
223	47.2	1187.6	-396.6	-365.7	11.8	20.7	205.27	122.9
223	57.0	1188.8	-403.5	-362.8	11.7	21.9	211.02	124.6
223	**68.5**	**1189.9**	**-383.7**	**-331.6**	**11.0**	**22.5**	**199.83**	**126.6**
223	78.5	1189.7	-377.2	-321.3	11.1	23.0	195.76	129.7
223	88.5	1189.2	-373.5	-312.9	11.3	23.1	191.87	132.4
241	47.2	1246.1	266.3	214.5	9.1	9.0	59.41	46.7
241	57.0	1246.3	300.6	247.5	10.4	9.7	70.06	44.0
241	**68.5**	**1246.5**	**324.4**	**266.7**	**11.5**	**9.9**	**75.66**	**41.5**
241	78.5	1246.3	295.6	233.3	11.5	8.8	62.59	38.2
241	88.5	1246.1	219.2	164.0	10.1	6.9	40.33	35.6
266	47.2	1314.8	128.3	86.0	5.6	5.0	15.56	33.7
266	57.0	1314.5	127.9	88.8	6.0	5.4	17.52	32.7
266	**68.5**	**1314.2**	**129.6**	**63.3**	**6.7**	**5.9**	**21.37**	**32.8**
266	78.5	1313.2	127.2	68.6	7.1	6.5	25.22	32.7
266	88.5	1311.7	125.3	75.3	7.6	7.3	30.64	33.5
327	47.2	1487.4	563.0	538.3	12.7	12.0	142.18	69.4
327	57.0	1487.5	546.8	527.0	13.1	11.8	139.64	64.3
327	**68.5**	**1487.5**	**538.9**	**529.2**	**12.8**	**12.4**	**139.52**	**61.2**
327	78.5	1487.3	512.1	508.4	12.1	13.2	135.08	58.0
327	88.5	1487.2	486.9	489.1	11.7	13.4	130.40	56.2
328	47.2	1488.3	-473.0	-499.3	11.6	12.1	132.87	109.1
328	57.0	1488.8	-460.9	-482.9	11.2	12.5	128.18	114.2
328	**68.5**	**1489.3**	**-456.8**	**-478.2**	**11.6**	**12.2**	**125.89**	**117.3**
328	78.5	1489.6	-443.8	-461.3	12.3	11.5	121.56	120.7
328	88.5	1489.9	-436.8	-449.6	12.5	11.3	118.34	122.8
335	47.2	1579.0	139.8	131.3	9.4	6.5	51.47	56.9
335	57.0	1578.8	133.1	127.2	9.8	6.5	52.09	54.4
335	**68.5**	**1578.3**	**133.7**	**130.7**	**9.7**	**7.2**	**55.14**	**51.5**
335	78.5	1578.1	130.1	128.1	9.4	7.8	54.98	48.1
335	88.5	1577.9	124.2	123.8	9.5	7.9	53.22	45.4
336	47.2	1581.3	-86.0	-107.8	5.4	8.7	37.88	125.9
336	57.0	1582.1	-83.6	-103.7	5.3	9.0	37.40	128.0
336	**68.5**	**1582.0**	**-90.6**	**-108.7**	**6.0**	**8.9**	**40.58**	**130.4**
336	78.5	1582.0	-95.1	-111.8	6.6	8.8	42.04	133.4
336	88.5	1581.8	-98.6	-113.5	6.7	9.1	42.70	136.1

Table S1: GCO analysis of the signature GCO-VCD bands in the linear transit structures using the GCO fragments defined in Figure 1a. Frequencies are given in cm^{-1}; R_{01} and $R_{01}^{\mathbf{GCO}}$ in 10^{-44} esu$^2\cdot$ cm^2; $|\vec{E}_{01}^{\mathbf{A}}|$ and $|\vec{E}_{01}^{\mathbf{B}}|$ in 10^{-20} esu$^2\cdot$ cm^2; $|\vec{E}_{01}^{\mathbf{A}} \times \vec{E}_{01}^{\mathbf{B}}|$ in 10^{-40} esu$^2\cdot$ cm^2; and τ and ξ in degrees.