SUPPORTING INFORMATION

Vibrational circular dichroism (VCD) methodology for the measurement of enantiomeric excess in chiral compounds in solid phase and for the complementary use of NMR and VCD techniques in solution: the camphor case

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SI1) Table with experimental wavenumbers (cm^{-1}) of the observed bands in the IR and VCD spectra of *R*-(+)-camphor in CCl_4 solution and solid phase (nujol mulls) and their assignment using the B3LYP/cc-pVDZ calculation according to the work of the reference 52 (J. R. Avilés Moreno *et al.*, *Asian J. Spectrosc.*, 2010, 14, 1–21).

MAIN SPECTRAL FEATURES[a]				
IR		**VCD**		**Assignment**
Wavenumbers, cm^{-1} (relative intensity)		**Wavenumbers, cm^{-1} (sign)**		
CCl_4	**Nujol**	**CCl_4**	**Nujol**	
1481 (w)	-	-	-	CH_2 sciss.
1470 (w)	-	1470 (+)	-	CH_2 sciss. + asym. CH_3 def.
1449 (m)	-	1453 (+) 1443 (-)	-	
1417 (m)	-	1417 (-)	-	CH_2 sciss.
1390 (m)	-	1390 (-)	-	sym. CH_3 def.
1372 (m)	-	1372 (-)	-	
1323 (m)	-	1323 (+)	-	CH rock. + asym. six member ring torsion + CH_2 wagg.
1299 (w)		1297 (-)	1297 (-)	CH rock. + asym. six member ring torsion + CH_2 wagg.
1277 (m)		1277 (+)	1277 (+)	CH def. + CH rock.
1256 (w)		-	-	-
1246 (w)		1245 (+)	1245 (+)	CH_2 twist. + CH_2 rock. + CH_2 wagg. + C-C str.
1219 (w)		1219 (-)	-	CH_2 twist. + CH def. + CH_2 wagg. + C-C str.
1197 (w)		1195 (-)	1195 (-)	CH def. + CH_3 rock. + CH_2 twist.
1166 (w)		1164 (+)	1167 (+)	CH def. + asym. six member ring torsion + CH_2 wagg.
1152 (vw)		1151 (-)	1152 (-)	C-C str.
1128 (vw)		1127 (+)	1128 (+)	CH_3 rock. + CH_2 twist. + C-C str.
1093 (w)		1093 (-)	-	CH_3 rock. + asym. six member ring torsion
1079 (w)		1079 (-)	-	CH_2 twist.
1045 (m)		1046 (-)	1046 (-)	C-C str. + trigonal six member ring def.
1021 (m)		1020 (-)	1020 (-)	C-C str. + CH_3 rock.
1010 (sh)		1010 (+)	1010 (+)	
978 (vw)	978 (w)	980 (-)	980 (-)	
951 (w)		948 (-)	949 (-)	
935 (w)		933 (+)	933 (+)	

925 (w)	925 (+)	925 (+)	C-C str. + CH_3 rock. + asym. six member ring torsion + CH_2 rock.
913 (vw)	912 (-)	912 (-)	trigonal six member ring def. + C-C str.

[a] s, strong; m, medium; w, weak; vw, very weak; sh, shoulder.

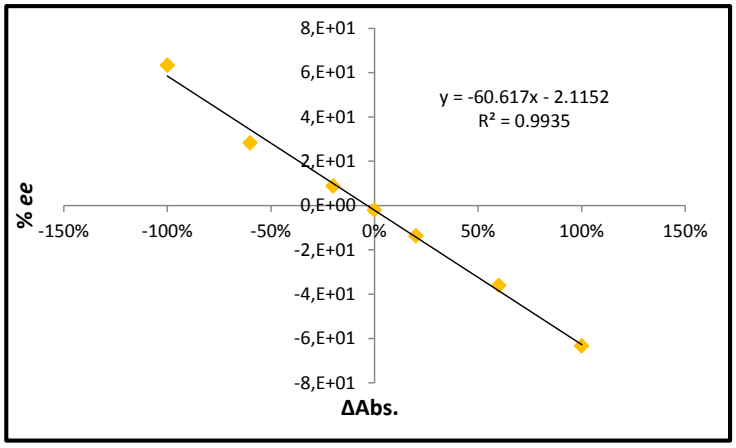
SI2) Linear regressions of the intensity of several VCD bands (ΔAbs.) *vs.* % *ee*

SI2a) IR-VCD spectra in CCl_4 solution

We have plotted the intensity of several VCD bands (ΔAbs.) *vs.* % *ee* and carried out a linear regression for each band. It can be seen that all the linear regressions show a good correlation coefficient (R^2) > 0.99, except one of the bands that shows a correlation coefficient of 0.986. The ΔAbs. values have been multiplied by 10^6 to have larger coefficients. We have also performed the interpolation of ΔAbs. of the blind sample for each band, obtaining the corresponding % *ee*.

Band at 1296.9 cm^{-1}

% *ee*	ΔAbs.
100	-63.32
60	-36.07
20	-13.70
-100	63.32
-60	28.26
-20	8.73
0	-2.03

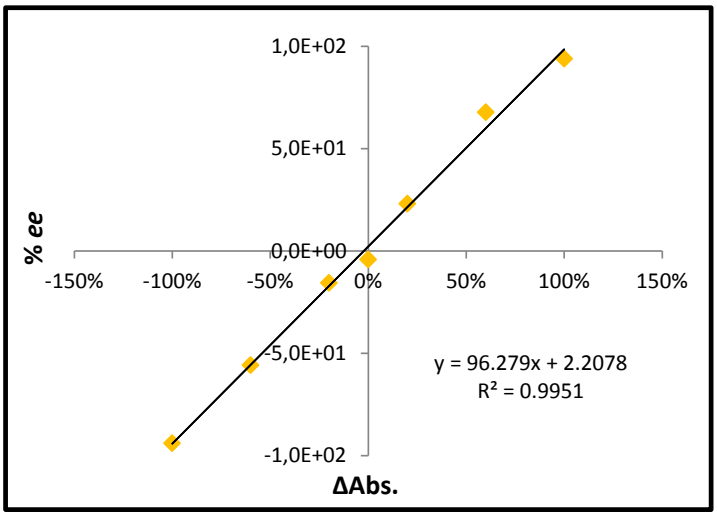


ΔAbs. (blind sample): -32.18

-32.18 = -60.617 x – 2.1152 → **x = % ee = 49.6**

Band at 1244.8 cm^{-1}

% *ee*	ΔAbs.
100	93.87
60	67.80
20	23.05
-100	-93.87
-60	-55.71
-20	-15.59
0	-4.10

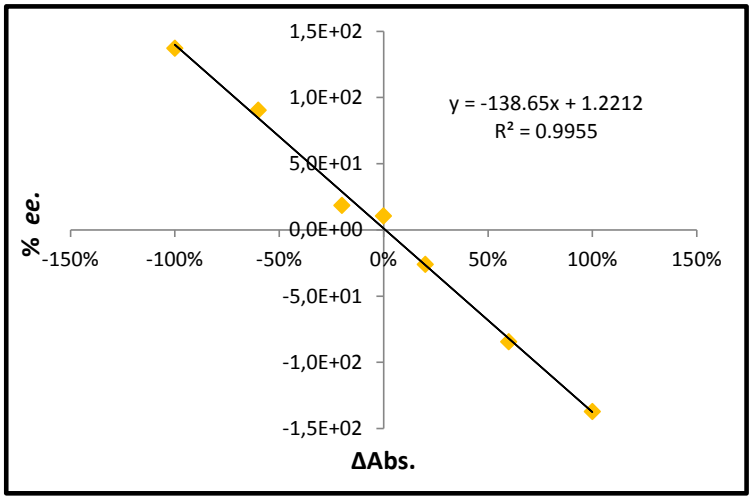


ΔAbs. (blind sample): 50.00

50.00 = 96.279 x + 2.2078 → **x = % ee = 49.6**

Band at 1046.2 cm^{-1}

% ee	ΔAbs.
100	-137.18
60	-84.49
20	-26.16
-100	137.18
-60	90.42
-20	18.38
0	10.41

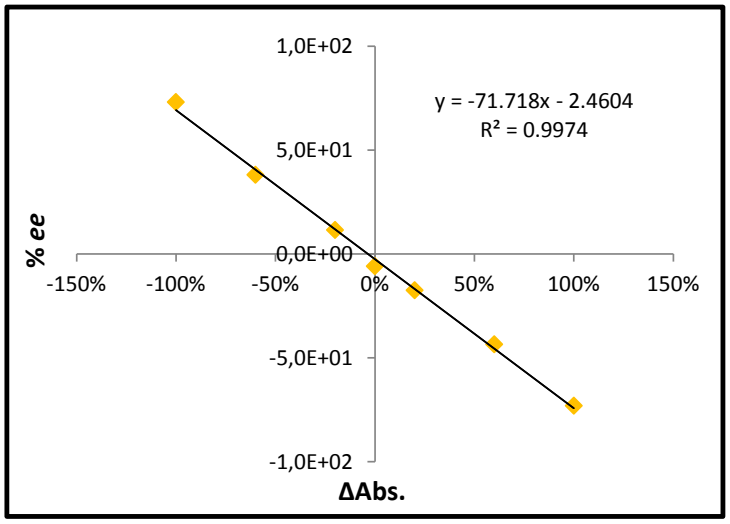


ΔAbs. (blind sample): -69.23

-69.23 = -138.65 x + 1.2212 → **x = % ee = 50.8**

Band at 947.8 cm^{-1}

% ee	ΔAbs.
100	-73.00
60	-43.53
20	-17.45
-100	73.00
-60	38.13
-20	11.58
0	-5.95

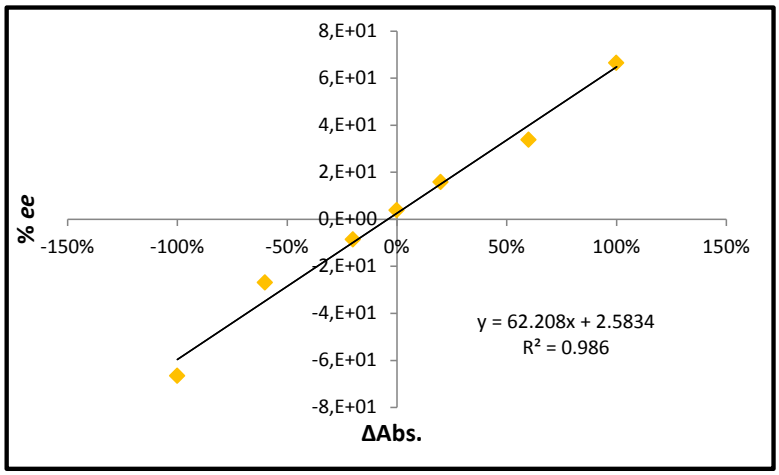


ΔAbs. (blind sample): -39.55

-39.55 = -71.718 x – 2.4604 → **x = % ee = 51.7**

Band at 933.4 cm^{-1}

% *ee*	ΔAbs.
100	66.47
60	33.78
20	15.80
-100	-66.47
-60	-26.85
-20	-8.54
0	3.89

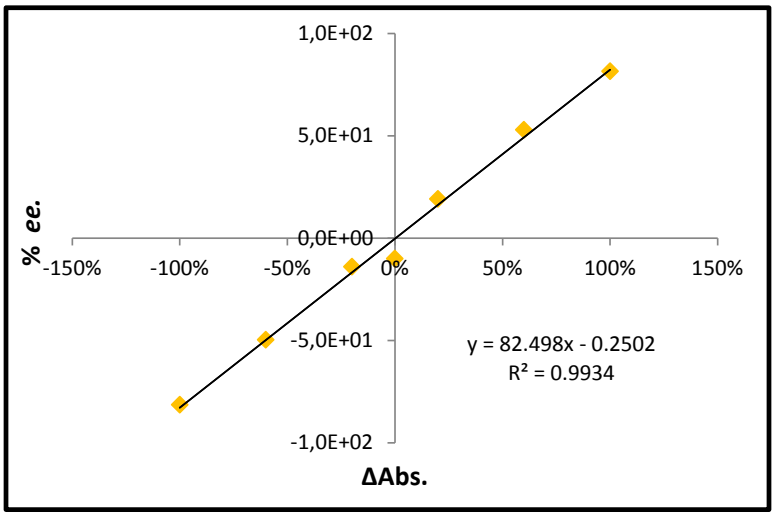


ΔAbs. (blind sample): 34.99

34.99 = 62.208 x + 2.5834 → **x = % ee = 52.1**

Band at 924.7 cm^{-1}

% *ee*	ΔAbs.
100	81.43
60	52.83
20	19.13
-100	-81.43
-60	-49.70
-20	-13.98
0	-10.03



ΔAbs. (blind sample): 41.24

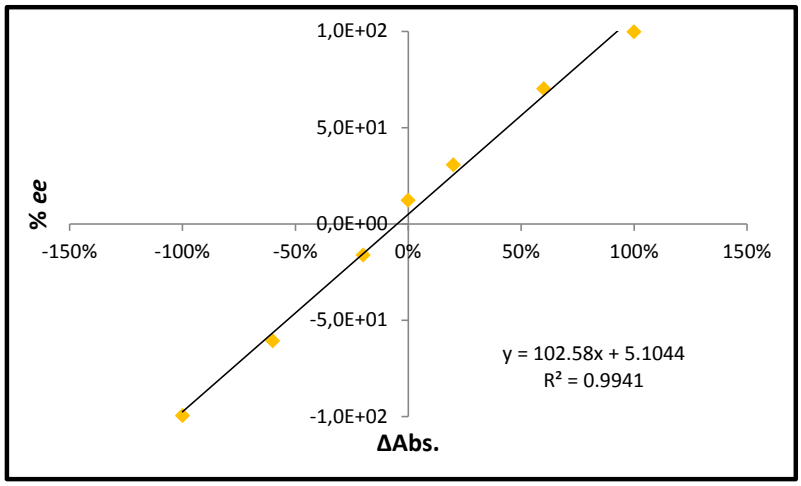
41.24 = 82.498 x – 0.2502 → **x = % ee = 50.3**

SI2b) IR-VCD spectra in nujol mull

We have also plotted the intensity of several VCD bands (ΔAbs.) *vs.* % *ee* and carried out a linear regression for each band. It can be seen that all the linear regressions show a good correlation coefficient (R^2) > 0,99.

Band at 1244.8 cm^{-1}

% *ee*	ΔAbs.
100	99.66
60	70.09
20	30.58
-100	-99.66
-60	-60.81
-20	-16.24
0	12.11

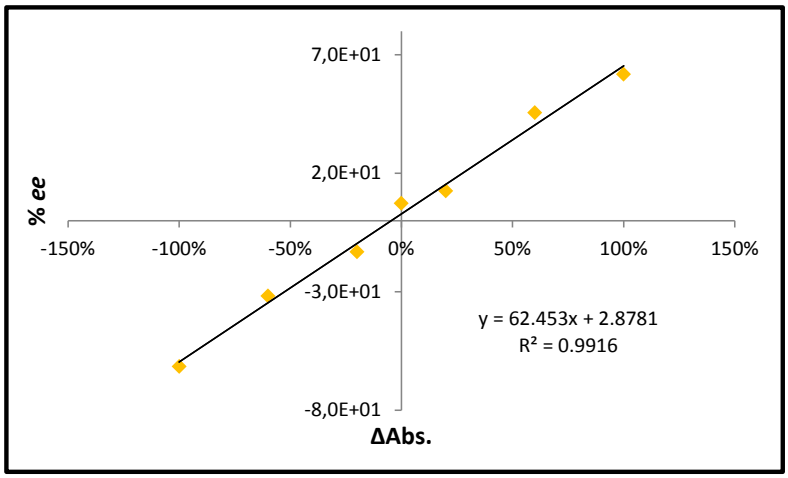


ΔAbs. (blind sample): 54.36

54.36 = 102.58 x + 5.1044 → **x = % ee = 48**

Band at 933.4 cm^{-1}

% *ee*	ΔAbs.
100	61.65
60	45.48
20	12.50
-100	-61.65
-60	-31.88
-20	-13.23
0	7.27

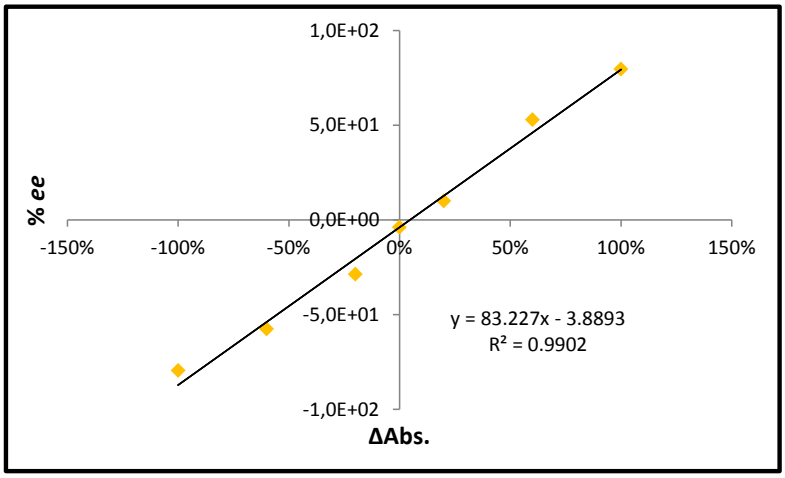


ΔAbs. (blind sample): 31.44

31.44 = 62.453 x + 2.8781 → **x = % ee = 45.7**

Band at 924.7 cm^{-1}

% *ee*	**ΔAbs.**
100	79.53
60	52.90
20	9.94
-100	-79.53
-60	-57.52
-20	-28.69
0	-3.85



ΔAbs. (blind sample): 38.04

38.04 = 83.227 x – 3.8893 → **x = % ee = 50.4**