Supporting Information C. M. Thiele, S. Berger: Probing the Diastereotopicity of Methylene-Protons in Strychnine Using Residual Dipolar Couplings

Table 1: Dependence of residual dipolar couplings $D_{C\text{-}H}$ of strychnine embedded in PBLG/$CDCl_3$ and of the quadrupolar splitting $\Delta\nu_Q$ of $CDCl_3$ from the static magnetic field B_0

B_0 /T	$\Delta\nu_Q$ / Hz	*D* C-14 / Hz	*D* C-13 / Hz	*D* C-20-H_a / Hz	*D* C-20-H_b / Hz	*D* C-16 / Hz	*D* C-8 / Hz	*D* C-12 / Hz	*D* C-4 / Hz	*D* C-1 / Hz	*D* C-22 / Hz
9.4	423	117.5	n.d[1]	70.1	n.d.[1]	n.d.[1]	n.d.[1]	113.0	-27.7	-21.1	n.d.[1]
14.1	454	129.0	n.d.[1]	89.0	n.d.[1]	-213.0	n.d.[1]	121.5	-17.7	-9.8	1.7
16.4	464	145.9	-38.5	105.7	-34.0	-209.0	-73.0	123.0	-15.0	-6.7	5.0

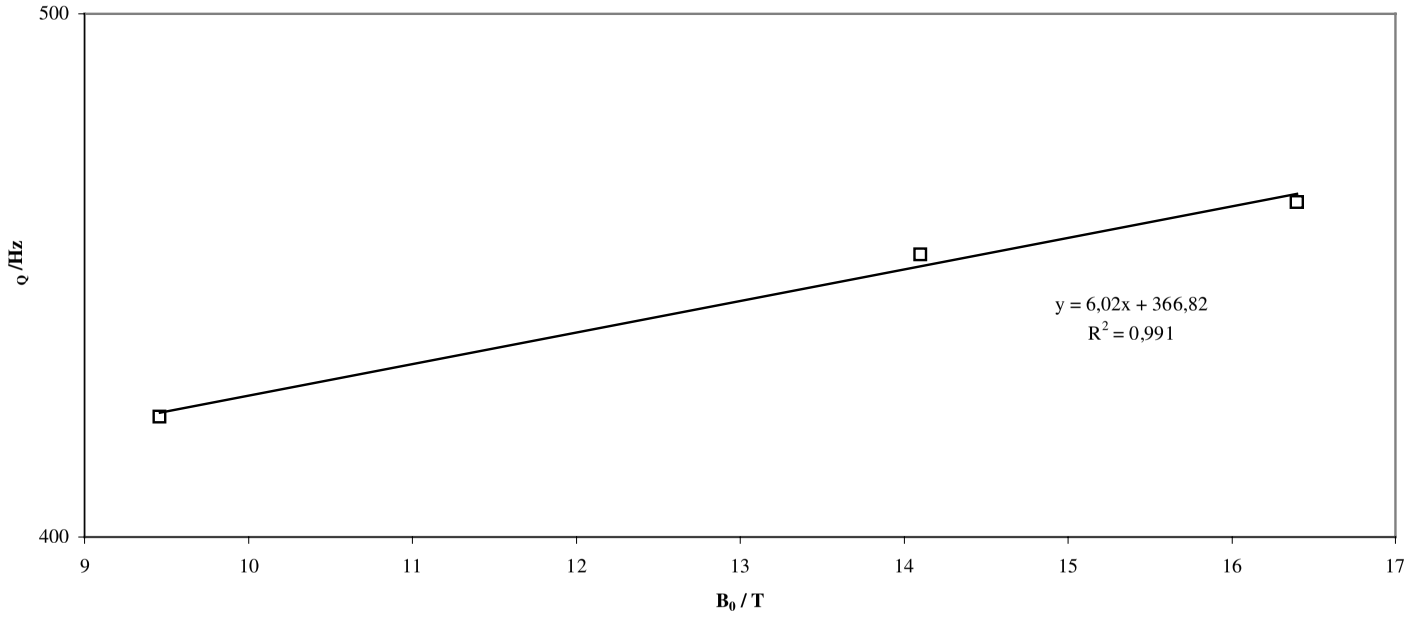


Figure 1: Dependence of the quadrupolar splitting $\Delta\nu_Q$ of $CDCl_3$ in PBLG from the static magnetic field B_0. Depicted as straight line with the corresponding equation and confidence limits.

[1] n. d. = not determined

Table 2: Comparison of observed residual dipolar couplings $D_{C\text{-}H}$ of strychnine embedded in PBLG/$CDCl_3$ and backcalculated ones D_{calc} (on the basis of the alignment tensor as performed within PALES[2]) for the right assignment of the two protons on C-20 on the left and for the wrong assignment on the right.

	right assignment of H_a and H_b on C-20		wrong assignment	
Residue	$D_{C\text{-}H}$ / Hz	D_{calc} / Hz	$D_{C\text{-}H}$ / Hz	D_{calc} / Hz
C1	-6.8	-13.4	-6.8	-15.2
C4	-15.6	-4.4	-15.6	-13.8
C12	123.0	116.2	123.0	127.3
C13	-42.3	-37.0	-42.3	6.1
C8	-75.5	-77.1	-75.5	-88.4
C22	4.3	-12.1	4.3	50.3
C14	123.8	133.0	123.8	122.6
C16	-209.6	-210.0	-209.6	-197.3
C20-1	98.7	95.7	-34.7	-23.1
C20-2	-34.7	-30.2	98.7	19.6

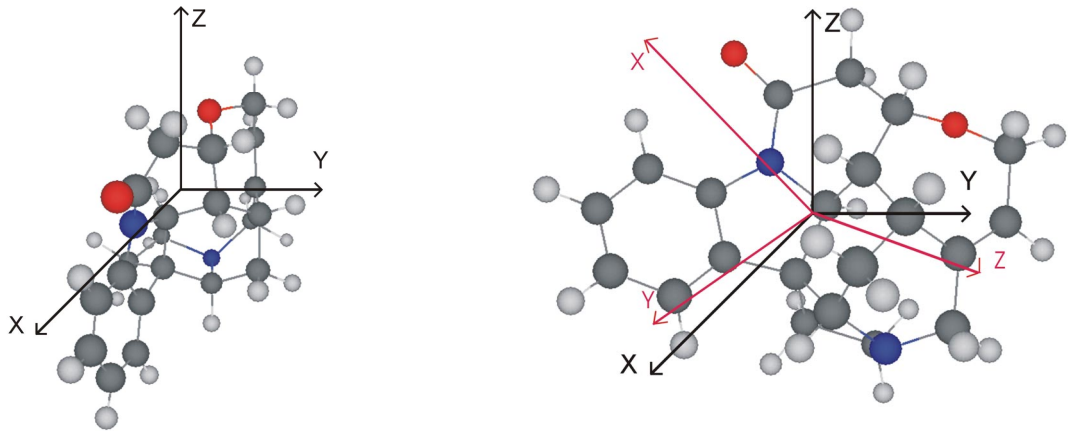
Table 3: Alignment tensor characteristics (as produced by PALES[2])

characteristic	value	standard deviation
S_{zz}	$4.7825 \cdot 10^{-3}$	$5.14 \cdot 10^{-5}$
G_{mag} / Hz	$1.74 \cdot 10^{2}$	1.78
$D_a = ½\ S_{zz}$	$-2.40 \cdot 10^{-3}$	
$D_r = 1/3\ S_{xx\text{-}yy}$	$-1.0 \cdot 10^{-3}$	
Rhombicity = D_r / D_a	0.42	

Table 4: Euler angles[3] (for rotation about x, y', z'') alpha, beta, gamma as produced by PALES[2]

alpha	beta	gamma
53	65	119
233	65	119
127	115	299
307	115	299

Figure 2: Rotation of the input pdb-file in such a way, that the alignment tensor coincides with the lab frame in black (left) as produced by PALES[2] and rotated in such a way that the orientation of the molecule within the magnetic field is shown (right). The labframe is depicted in black, the alignment tensor in red[4].



[2] Zweckstetter, M.; Bax, A. *J. Am. Chem. Soc.* **2000**, *122*, 3791-92.
[3] Four equivalent orientations are reported due to the sign ambiguity of the eigenvectors.
[4] only one orientation depicted