

Enhanced Measurement of Residual Chemical Shift Anisotropy for Small Molecule Structure Elucidation

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Introduction to the PBLG Liquid Crystal Medium

The phase transition and the texture of the cholesteric phase of PBLG have been thoroughly studied by microscopy and X-ray diffraction as described.¹⁻³ Briefly, at a low [PBLG], the solution is isotropic. When [PBLG] is higher than a critical concentration A, two phases co-exist in equilibrium including a heavier isotropic phase and a polymer-enriched mesophase characterized by a periodic multi-layered supramolecular structure. Increasing [PBLG] beyond A converts more isotropic phase to mesophase with polymer concentrations in both phases staying constant, until [PBLG] reaches a second critical concentration B at which point the whole sample goes into mesophase; at an even higher [PBLG], the supramolecular packing density increases proportionally. The concentration gap between A and B is typically small for high-molecular weight PBLG and in this work we only utilize [PBLG] below A and above B for extraction of RCSA. If a biphasic solution is encountered, which can be revealed by an inhomogeneous ²H spectrum of CDCl₃ showing one pair of signals separated by residual quadrupolar coupling (RQC) of several hundred Hz and a singlet or a pair of signals with barely resolved RQC, as described in ref 19 in the main text, a small amount of additional PBLG should be added until only the pair with a large RQC are observed.

Experimental Procedures

Sample Preparation

Strychnine: Strychnine (30mg, MP Biomedicals, Inc.) was dissolved with 600 μ L of CDCl₃ in a 5 mm NMR tube. Tetramethylsilane (TMS) of 4% (v/v) was added for RCSA referencing. Carbon chemical shifts and ¹³C-¹H *J* couplings were measured. Poly- γ -benzyl-L-glutamate (PBLG, 150,000-350,000 Da, Sigma-Aldrich catalog No.: P5136) was successively added to afford weight-to-volume ratios of 2.1%, 4.1%, 6.6%, 8.8%, 11.4%, 12.9%, 15.5%, 18.4%, 22.9%, and 34.5%, and after each addition, carbon chemical shifts were measured, as described in the main text. The ²H spectrum of CDCl₃ was taken at each PBLG concentration to measure the residual quadrupolar coupling (RQC). The common method to dissolve PBLG is to briefly and repeatedly centrifuge the NMR tube with interleaved tube inversions, until a clear and homogenous solution was obtained.⁴ Solid PBLG is lighter than CDCl₃; therefore by repeatedly inverting the NMR tube followed by centrifugation, the undissolved PBLG moves across the sample solution from one end to the other as it dissolves, creating a homogenous PBLG solution. See more details in the section of "Step-by-Step Procedure of NMR Sample Preparation".

Retrorsine: A sample of 10mg retrorsine (Sigma-Aldrich, Inc.) was prepared in the same fashion as for the strychnine sample, but with the successive addition of 0%, 8.1%, 12.6%, and 15.1% PBLG. TMS of 2.5% (v/v) was added for RCSA referencing. Carbon chemical shifts and CDCl₃ RQC were measured after each PBLG addition.

Caulamidine A: A sample of 1.6mg caulamidine A was dissolved in 170 μ L CDCl₃ with 5 μ L TMS in a 3mm NMR tube. The material was quantified by external calibration with another sample of 3.6 mg 1,3,5-trimethoxybenzene (TMB) dissolved in 170 μ L CDCl₃, through comparison of the ¹H integration of caulamidine A or TMB over that of the residual CHCl₃ signal. RCSA was measured with 10 of no PBLG, 11 of 6.3% PBLG, and A1 of 13.1% PBLG. Carbon chemical shifts and CDCl₃ RQC were measured after each PBLG addition.

NMR Experiments

All NMR data were acquired on a Bruker 600 MHz spectrometer equipped with a helium cooled cryoprobe with the sample temperature maintained at 25 °C. For the measurement of carbon chemical shifts, the standard {¹H}-¹³C experiment was employed with a 90° flip angle, a recycling delay of 2 s, and an acquisition time of 2 s, unless otherwise noted. Strychnine and retrorsine spectra were acquired with 32 and 64 transients, respectively, at all PBLG concentrations. As described in the main text, a higher decoupling field is needed to fully collapse large ¹³C-¹H RDCs as the alignment gets stronger: for strychnine, proton decoupling was conducted using WALTZ16 with a decoupling field of 3125 Hz for the samples of 0%, 2.1%, 4.1%, 6.6%, and 8.8% PBLG in which the samples were isotropic; after alignment was induced at higher PBLG concentrations, proton decoupling was performed using WALTZ16 with a decoupling field of 4167 Hz for the sample of 11.9% PBLG; GARP with a decoupling field of 4167 Hz was used for the samples of 12.9%, 15.5%, and 18.4% PBLG, and GARP with a decoupling field of 8333 Hz was used for the samples of 22.9% and 34.5% PBLG. For retrorsine, proton decoupling was performed using WALTZ16 with a decoupling field of 3125 Hz for samples of 0% and 8.1% PBLG in which the samples were isotropic. GARP with a decoupling field of 4167 Hz was employed for the samples of 12.6% and 15.1% PBLG in which the samples were aligned. Carbon spectra of caulamidine A were collected with 800, 1024, and 3072 transients for 0%, 6.3%, and 13.1% PBLG, respectively. The acquisition time was 0.5 s for caulamidine A with 13.1% PBLG. Proton decoupling was performed with WALTZ16 with a decoupling field of 4167 Hz for 0% and 6.3% PBLG, and GARP with a decoupling field of 4167 Hz for 13.1% PBLG.

DFT Calculation

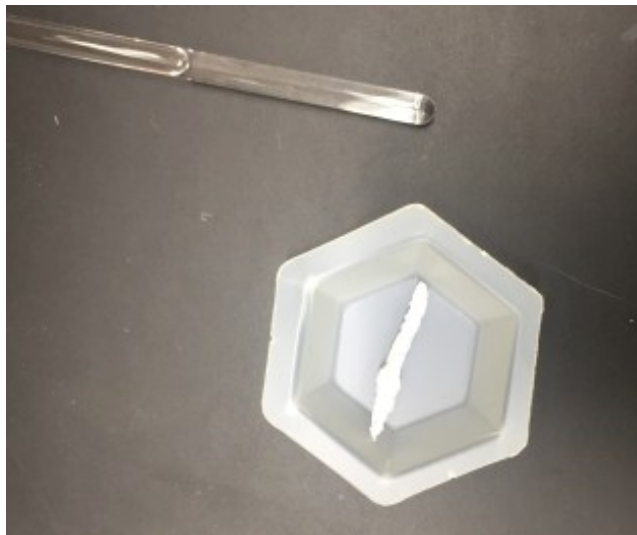
The density functional theory (DFT)-computed coordinates and chemical shielding tensors of strychnine and its twelve other diastereomers were adopted from a previous publication.⁵

For retrorsine, the initial conformers were collected by combining outputs from three different conformer search programs including ET⁶, JG (a Merck in-house version of DG⁷), and OpenEye's OMEGA⁸, and were further optimized by DFT in Gaussian 09⁹ at the B3LYP/6-31G(d,p) level in the gas phase. The chemical shielding tensors were calculated in Gaussian 09 with the "nmr" keyword at the mPW1PW91/6-31G(d,p) level.

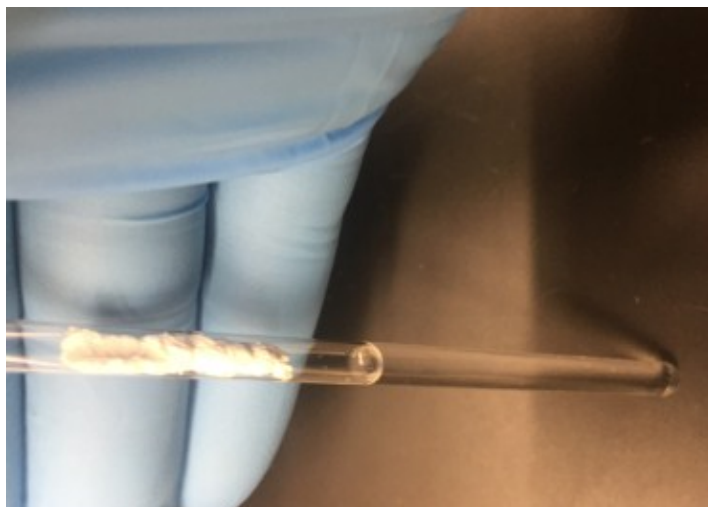
DFT calculation on caulamidine A was performed by a similar procedure as for retrorsine, as reported in Ref 11 of the main text.

Step-by-Step Procedure for NMR Sample Preparation

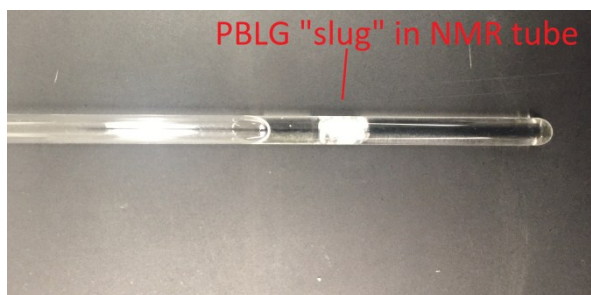
1. Transfer the sample to a ~5.0 mL glass vial, and dissolve with 0.6 mL CDCl_3 .
2. Transfer the solution to a 5-mm NMR tube.
3. Weigh the desired amount of PBLG, and roll by hand into a thin rod.



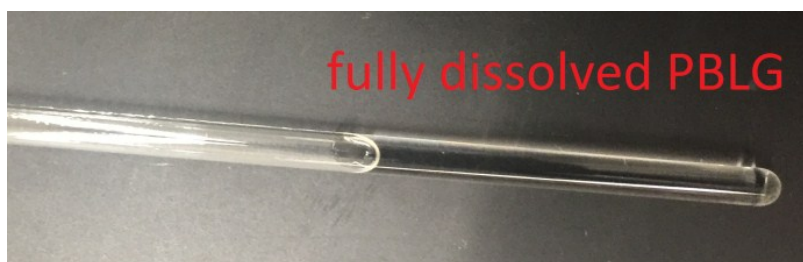
4. Directly insert the rolled PBLG into the NMR tube and cap with a standard NMR tube cap, e.g. New Era P/N NE-310-5 or comparable. To minimize chloroform evaporation, the cap is wrapped with Parafilm M®.



5. Dissolve the PBLG by repeatedly inverting and centrifuging the tube. The PBLG will become a viscous "slug" within the tube. The PBLG "slug" can then be spun back and forth across the sample solution using a low-speed centrifuge, until it fully dissolves. From 20 to 30 inversions may be necessary to fully dissolve the PBLG for a homogenous sample, which takes about 10 mins. A fixed angle rotor is the ideal option for spinning the NMR tube. If a variable angle rotor is used as in our case, it is important to make sure that the NMR tube is shorter than the maximal rotation radius (r_{MAX}) so that the entire sample volume moves back and forth under centrifugation as the NMR tube is inverted.

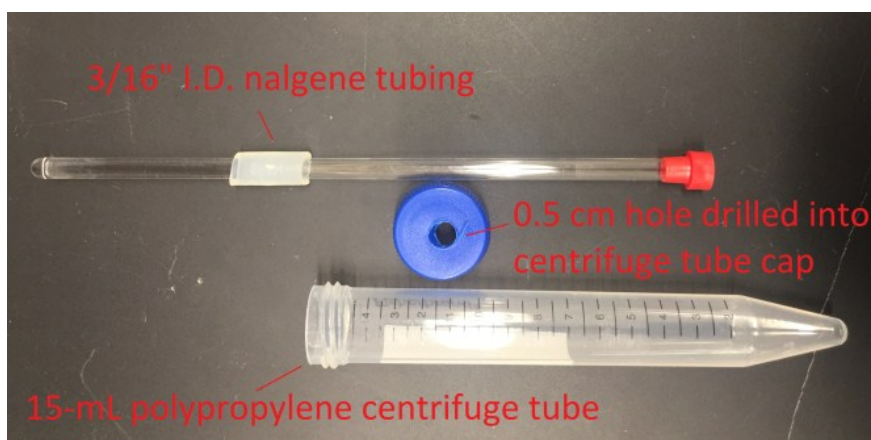


6. When the PBLG is fully dissolved, the solution will be clear.

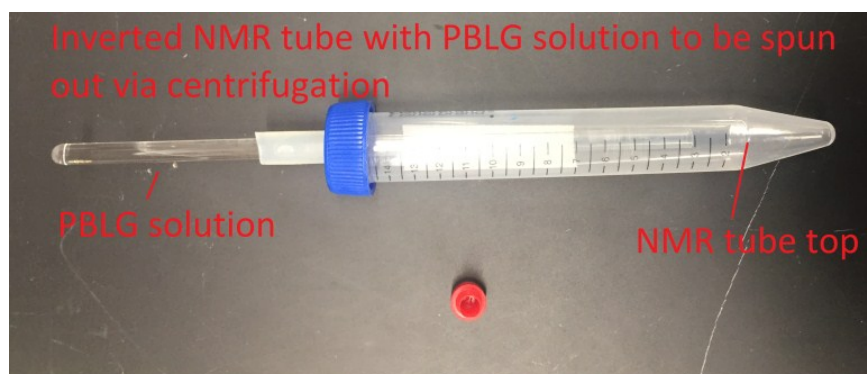


Step-by-Step Procedure for NMR Sample Recovery

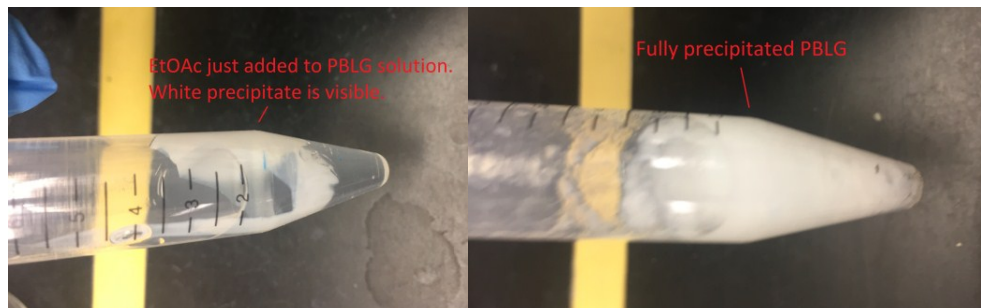
1. This sample recovery method is based on insolubility of PBLG in ethyl acetate (EtOAc). Conversely, the sample to be recovered *must* be soluble in EtOAc. If this is not the case, then chromatographic recovery (e.g., size exclusion chromatography) may be feasible.
2. The PBLG solution is quite viscous so it should be spun out of the tube using a centrifuge. First, cut a 0.5 in. piece of 3/16 in. I.D. Nalgene® tubing, which will fit snugly around the 5 mm NMR tube. Drill a 0.5 cm hole in the top of a 15 mL conical bottom polypropylene centrifuge tube (Fisherbrand, P/N 05-539-12). Pre-rinse the centrifuge tube twice with EtOAc to remove any contaminants (e.g., plasticizer).



3. Insert the NMR tube into the centrifuge tube upside down and with the Nalgene® tubing "stopper" at the top such that the open end of the NMR tube just touches the beginning of the conical taper. Be sure to leave enough room below the open end of the NMR tube so that the sample solution spun out does not contact the tube opening.



- Gently spin out the PBLG solution using a centrifuge. Rinse with 1-2 mL CDCl_3 followed by EtOAc to recover sample from the walls of the NMR tube, and continue to spin out each time using a centrifuge.
- Concentrate the solution in the centrifuge tube under a stream of dry N_2 gas. Periodic agitation may be needed as the PBLG may form a film on top of the solution.
- Add approximately 10 mL of EtOAc to precipitate the PBLG. The precipitation may be aided by vortexing. Further concentrate the solution down to 5 mL, which should fully remove residual CDCl_3 .



- Rinse a 1.0 μm PTFE filter (Whatman Puradisc® 25 TF) and 5 mL plastic Luer-lock syringe with EtOAc to remove contaminants.
- Centrifuge the precipitated solution in the centrifuge tube, and filter the supernatant into a 5 mL glass vial. Repeat by washing the filtrate 1-2 times more with EtOAc to ensure thorough sample recovery.
- The EtOAc can then be simply removed under a stream of dry N_2 gas.

Summary of Sample Recovery Results

The sample recovery procedure was initially optimized on ibuprofen and then tested for seven additional small molecule compounds: fluconazole, acetanilide, lidocaine, trimethoprim, avobenzene, benzocaine, carbamazepine (all compounds purchased from Sigma-Aldrich as certified reference standards). Recovery was based on the insolubility of PBLG in ethyl acetate. Most small molecules that are soluble in chloroform are also soluble in ethyl acetate. However, in cases where the compound to be recovered is insoluble in ethyl acetate, then chromatographic separation is recommended. The key to high recovery is ensuring that the viscous PBLG solution can be fully transferred between the NMR tube and centrifuge tube for precipitation with ethyl acetate. Several rinses with both chloroform and ethyl acetate were found to improve recovery from ~60% to >90%. Fig S1 shows the spectrum of ibuprofen before and after recovery. A small amount of extractable plasticizer (dioctyl phthalate) was also initially observed. This was traced to the plastic syringe barrel and could be minimized by pre-rinsing the syringe with ethyl acetate or by using glass Luer-lock syringes. Simultaneous recovery of all eight tested compounds was found to be greater than 90% as measured by quantitative NMR. For the qNMR measurement, 1,3,5-trimethoxybenzene (TMB) was used as internal standard, and a relaxation delay of 60 s was used with a tip angle of 30° . The 6.1 ppm aromatic signal of TMB did not interfere with any sample component signals and was thus utilized for quantitation. The resolved signals of each compound used for quantitation were as follows: fluconazole, 8.06 ppm, s, 2H; acetanilide, 2.17 ppm, s, 3H; lidocaine, q, 4H; trimethoprim, 6.38 ppm, s, 2H; avobenzene, 7.97 ppm, d, 2H; ibuprofen, 7.21 ppm, d, 2H; benzocaine, d, 6.63 ppm, 2H; carbamazepine, 6.93 ppm, s, 2H.

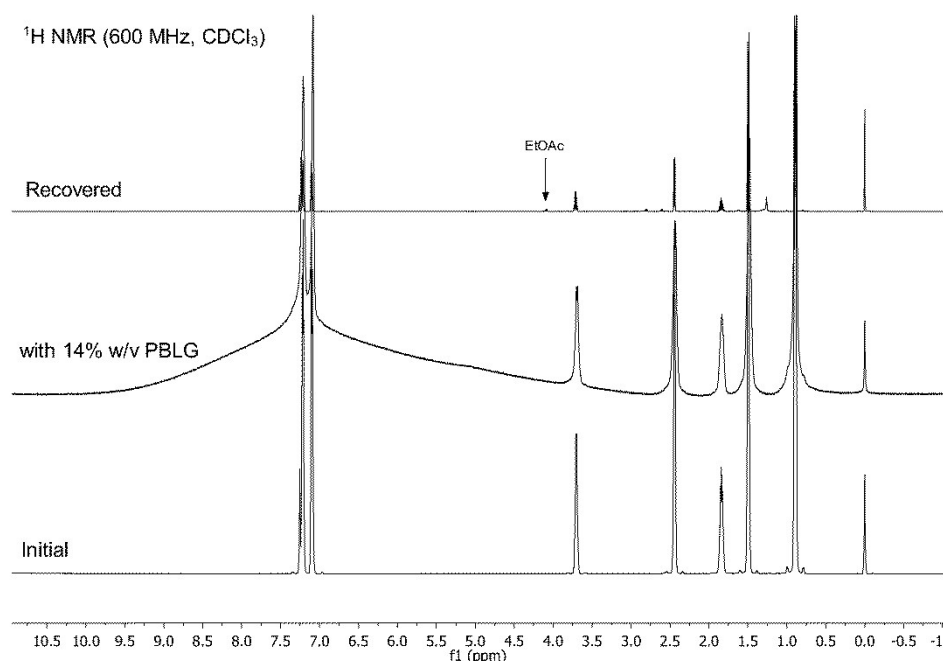


Figure S1. NMR spectra from the initial sample recovery test with ibuprofen. Note that the broad PBLG signal centered around 7.2 ppm completely disappeared after recovery. Although the recovery rate of this initial test was estimated to be only ~60%, the improved procedure achieved a 94.9% recovery rate (Table S1) by fully transferring the viscous PBLG sample from the NMR tube to the centrifugation tube.

Table S1. Sample recovery from PBLG solutions

Compound	MW (g/mol)	Purity (%)	Initial Wt (mg)	Recovered Wt (mg)	Recovery (%)
fluconazole	306.3	99.6	2.54	2.38	93.6
acetanilide	135.2	99.9	2.62	2.40	91.7
lidocaine	234.3	99.8	3.79	3.62	95.6
trimethoprim	290.3	99.8	4.65	4.44	95.5
avobenzene	310.4	99.9	4.52	4.28	94.6
ibuprofen	206.3	99.9	4.43	4.21	94.9
benzocaine	165.2	99.9	4.23	4.02	95.0
carbamazepine	236.3	99.9	3.83	3.81	99.4

Results and Discussion

The ^1H and ^{13}C spectra under Strong Alignment Conditions

With strong alignment in the PBLG mesophase, the homonuclear RDCs introduce an extensively coupled network and cause severe line-broadening of the ^1H spectrum. As shown in Fig S2a, in going from 0% to 8.1% PBLG, both of which were isotropic based on the absence of CDCl_3 RQC (Fig S2b), the increase in ^1H line-width was very modest. However, increasing the PBLG concentration to 12.6% caused a transition to the mesophase, as indicated by a CDCl_3 RQC of 272.6 Hz (Fig S2b), which was accompanied by substantial ^1H line-broadening due to the emergence of RDCs; such broadening was more pronounced with even stronger alignment at 15.1% PBLG (CDCl_3 RQC = 406.5 Hz). In contrast, as shown in Fig S2c, in the ^{13}C spectrum both the inhomogeneous broadening and homogenous broadening due to proton spin diffusion can be largely suppressed by proton decoupling, and therefore the line-width increase in PBLG mesophase is much less severe for ^{13}C than for ^1H . The sharp ^{13}C resonances facilitate accurate RCSA measurement even at high degrees of alignment. Also note that except for the two broad signals between 132 and 134 ppm (Fig S2c expansion to the left), other background ^{13}C signals from the PBLG LC medium is extremely weak, yielding very clean spectra.

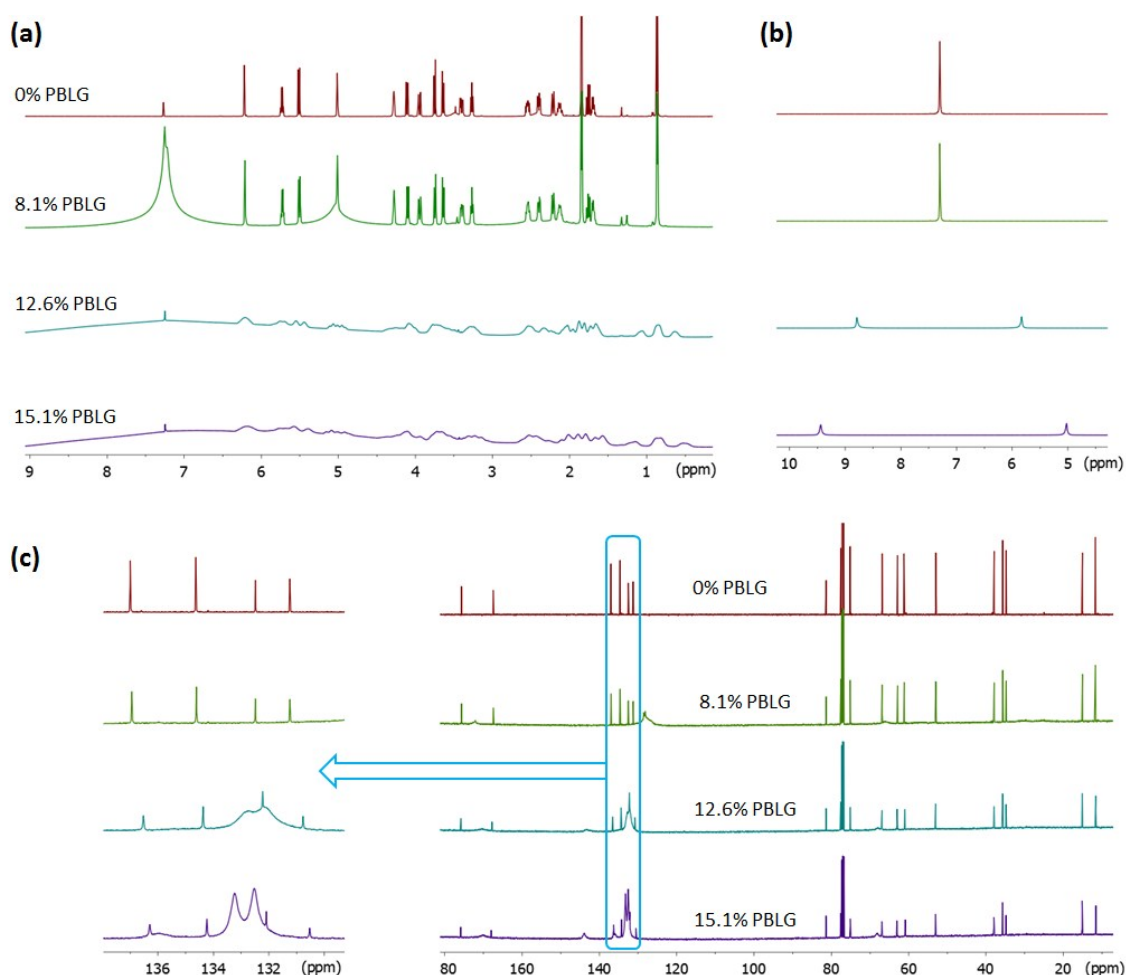


Figure S2. ^1H (a) and $^{13}\text{C}\{^1\text{H}\}$ (c) spectra of retrorsine and ^2H (b) spectrum of CDCl_3 at different PBLG concentrations.

Rationale and Limitation of the $\Delta\Delta\delta_{\text{iso}}$ Correction Method

Our correction method is based on the premise that the $\Delta\Delta\delta_{\text{iso}}$ dependence on PBLG concentration is identical in both phases, such that the $\Delta\Delta\delta_{\text{iso}}$ in the mesophase can be corrected for by extrapolating its value from its trend in the isotropic phase. This assumption is reasonable because of two points. First, the analyte can diffuse freely through the highly fluidic mesophase,¹⁻³ and second, $\Delta\Delta\delta_{\text{iso}}$ is determined to the first order by the total surface area of PBLG polymers from averaging all microstates of the analyte with orientational and positional degrees of freedom at the intermolecular interface. An effect not considered, however, is the interference between different surfaces on neighbouring PBLG molecules, which can become relevant with increasing PBLG concentration. This effect can, for instance, reduce the accessible area when two PBLG surfaces are very close or alter the microstates of an analyte trapped between two surfaces. It is noteworthy that the orientational redistribution of PBLG during the phase transition, while generating RCSA, is not expected to cause $\Delta\Delta\delta_{\text{iso}}$ by itself, although associated changes in surface interference may. However, as our studies in this work demonstrate, ignoring the interference does not cause significant errors to RCSA measurement.

Correction for $\Delta\Delta\delta_{\text{iso}}$ in RCSA measurement

As shown in Fig S3, the TMS-referenced isotropic carbon chemical shift (^{13}C $\Delta\Delta\delta_{\text{iso}}$) approximately follows a linear relationship as a function of PBLG concentration when the concentration is below the critical LC forming concentration. As described in the main text, this linear dependence forms the basis for the ^{13}C $\Delta\Delta\delta_{\text{iso}}$ correction used in the I0-I1-A1 method for RCSA measurement. Note that the ^{13}C $\Delta\Delta\delta_{\text{iso}}$, as shown in Fig S3, is quite small in comparison to ^{13}C RCSA (See Table S1).

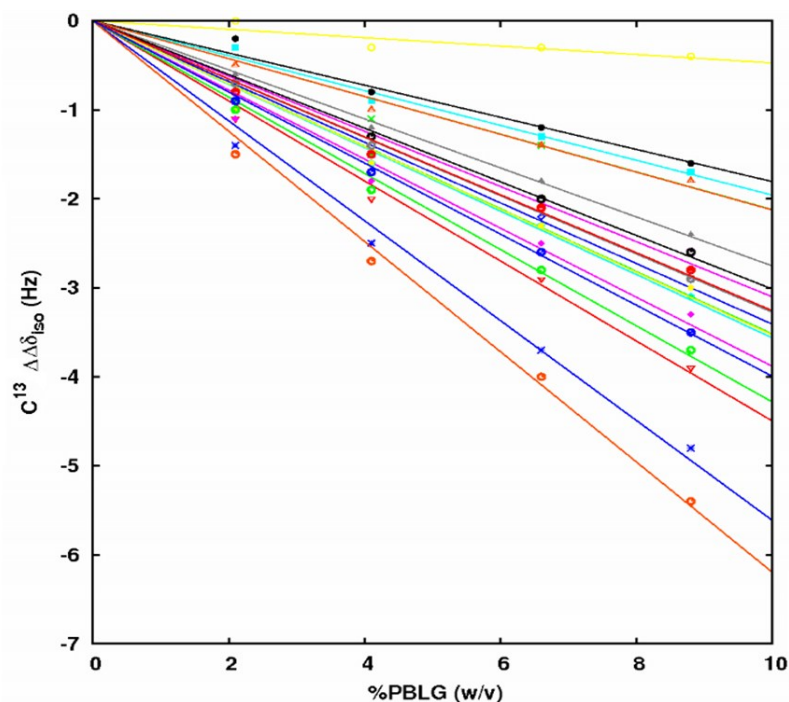


Figure S3. ^{13}C $\Delta\Delta\delta_{\text{iso}}$ of strychnine as functions of PBLG concentration. The curves were fitted to $y=a*x$ through linear regression. Curves for all 21 carbons of strychnine are displayed. Data were acquired on a 600 MHz spectrometer. Chemical shifts were internally referenced to TMS.

Effects of insufficient ^1H -decoupling in Strongly Aligned Samples

The potentially large and extensive ^{13}C - ^1H RDCs observed for strongly aligned molecules may exceed the default ^1H decoupling capability commonly used for solution NMR experiments. As shown in Fig S4a (top trace), the default ^1H decoupling by WALTZ16 with a decoupling field of 3125 Hz led to the residual multiplet structure for C23 of strychnine aligned in 11.9% PBLG (Refer to Fig 1a in the main text for atomic numbering), whereas increasing the decoupling field to 4167 Hz collapsed the multiplet (Fig S4a, bottom trace); with an even stronger alignment at 12.9% PBLG, C23 showed up again as a residual multiplet with 4167 Hz WALTZ16 (Fig S4b, top trace). Switching from WALTZ16 to GARP yielded better off-resonance decoupling efficiency at the same decoupling power and restored the singlet (Fig S4b, bottom trace).

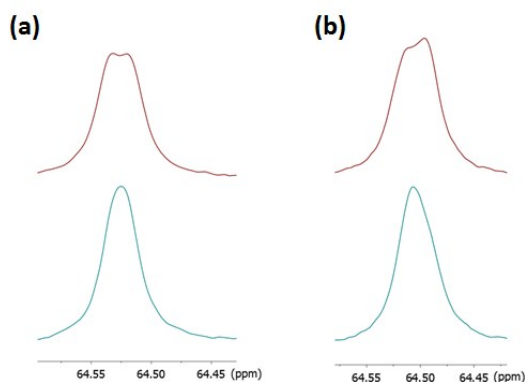


Figure S4. Spectral effects of insufficient ^1H -decoupling in the presence of large RDCs in strongly aligned PBLG mesophase. (a) & (b): Red and blue spectra were acquired with insufficient and sufficient ^1H -decoupling, respectively.

Experimental RCSA Data of Strychnine

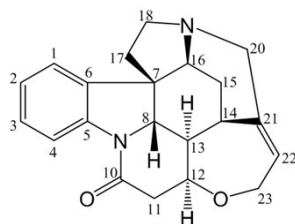


Table S2. Experimental RCSA data (in Hz^a) of strychnine after correction for $\Delta\Delta\delta_{iso}$ in various PBLG mesophases.

	[PBLG] (w/v)					
	11.4%	12.9%	15.5%	18.4%	22.9%	34.5%
C10	26.8	35.8	50	65.4	92.6	158.9
C5	29.3	39.5	55.9	73.3	104.9	181.8
C21	34.9	46.7	65.1	84.2	116.6	187
C6	45.4	61.3	86.6	113.7	N/A ^b	281.2
C3	52.2	70.3	99.2	130.3	186.2	324.1
C22	23.8	31.6	43.5	55.9	76.3	119
C2	45.4	61.1	86	112.7	160.2	275.5
C1	67.2	90.5	127.3	166.4	235	396.2
C4	59.2	79.7	112.1	146.5	207.8	353.1
C12	1.8	2.1	2.5	2.9	3.7	4.8
C23	-6.2	-8.6	-14.3	-18	-26.5	-46.8
C16	-2.4	-3.5	-5.3	-7.3	-10.5	-18.7
C8	-14.3	-19.8	-28.1	-36.9	-52.4	-88.9
C20	1.3	2	2.6	0.9	1.9	1.7
C7	-3.4	-5.1	-7.5	-10	-14.6	-25.7
C18	13.6	18.2	25.2	32.7	45.8	76.5
C13	0.4	0.1	-0.6	-1.1	-2.3	-5.4
C17	6.4	8.6	11.8	15.4	22	38.3
C11	-4.7	-6.8	-9.9	-13.5	-19.6	-36.5
C14	2.8	3.6	4.8	6	8.3	14
C15	-6.7	-9.4	-13.6	-17.9	-25.5	-43.4
CDCl₃ RQC	215.5	286.4	394.9	505.6	687.4	1084.2

[a] Values in Hz are based on a spectrometer frequency of 600 MHz. [b] Data not available due to overlap with PBLG benzyl signals.

Experimental RCSA Data of Retrorsine

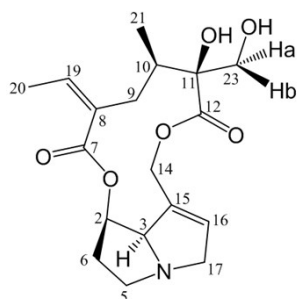


Table S3. Experimental RCSA data (in Hz^a) of retrorsine after correction for $\Delta\Delta\delta_{\text{iso}}$ in PBLG mesophases.

	[PBLG] (w/v)	
	12.6%	15.1%
C12	19.8	29.6
C7	54.4	82.4
C16	-58.3	-90.4
C19	-35.2	-55
C8	-39.9	-59.5
C15	-71.7	-107.2
C11	4.1	7.2
C3	9.3	13.1
C2	-1.4	-3
C23	5.2	9
C17	19.5	29.7
C14	-21.6	-35.7
C5	8.5	12.9
C9	4.6	7.5
C10	9.9	14.9
C6	7.9	11.7
C20	6.8	9.9
C21	-8.2	-13.1
CDCl₃ RQC	272.6	406.5

[a] Values in Hz are based on a spectrometer frequency of 600 MHz.

Experimental RCSA Data of Caulamidine A

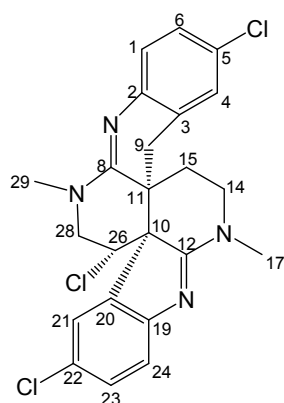


Table S4. Experimental RCSA data (in Hz^a) of caulamidine A after correction for $\Delta\Delta\delta_{\text{iso}}$ in PBLG mesophases.

	[PBLG] (w/v)
	13.1%
C12	33.5
C8	42.1
C19	3.6
C2	53.3
C20	N/A ^b
C23	-11.7
C6	102.9
C22	-3
C5	12.5
C4	53.6
C1	60.1
C3	96.2
C21	38.7
C24	33.7
C10	4.6
C26	-15.6
C28	-41.2
C14	-36.2
C11	-2.5
C17	-20.7
C29	-10.3
C9	-5
C15	4.9
CDCl₃ RQC	385.7

[a] Values in Hz are based on a spectrometer frequency of 600 MHz.

[b] Resonance of C20 overlapped with the benzyl signals of PBLG and could not be reliably interpreted.

Structure Coordinates and Chemical Shielding Tensors of Strychnine from DFT computation

Refer to supporting information from Ref 5.

Structure Coordinates of Retrorsine from DFT Geometry Optimization

Conformer 1

C	2.234	-0.125	1.162
C	3.684	0.344	0.978
C	4.120	-0.378	-0.305
N	3.438	-1.675	-0.239
C	2.344	-1.613	0.762
C	2.928	-2.238	-1.494
C	1.530	-2.672	-1.155
C	1.188	-2.321	0.088
O	1.345	0.537	0.228
C	1.050	1.841	0.478
C	0.062	2.370	-0.516
O	1.534	2.463	1.405
C	0.142	3.636	-0.965
C	1.145	4.696	-0.626
C	-1.030	1.418	-0.955
C	-2.024	1.102	0.200
C	-0.089	-2.691	0.775
O	-1.043	-1.586	0.853
C	-1.797	-1.384	-0.232
C	-2.790	-0.222	-0.066
O	-1.727	-2.032	-1.261
C	-2.973	2.288	0.426
O	-3.544	-0.145	-1.273
C	-3.785	-0.595	1.052
O	-4.413	-1.829	0.754
H	2.628	-2.153	1.683
H	1.920	4.342	0.052
H	1.606	5.086	-1.542
H	0.643	5.546	-0.147
H	-3.684	2.370	-0.401
H	-3.538	2.197	1.358
H	-2.401	3.219	0.483
H	4.271	-0.008	1.833
H	3.772	1.429	0.932
H	5.209	-0.494	-0.364
H	3.803	0.197	-1.192
H	3.540	-3.082	-1.848
H	2.928	-1.494	-2.310
H	-0.569	0.497	-1.322
H	-1.586	1.851	-1.792
H	0.082	-2.955	1.822
H	-0.576	-3.523	0.264
H	-4.521	0.213	1.154
H	-3.263	-0.716	2.005
H	1.853	0.035	2.173
H	-1.442	0.937	1.115
H	0.890	-3.211	-1.846
H	-0.614	3.934	-1.692
H	-3.113	-0.766	-1.888
H	-4.758	-1.720	-0.146

Conformer 2

C	2.277	-0.127	1.121
C	3.718	0.335	0.867
C	4.096	-0.408	-0.422
N	3.428	-1.707	-0.297
C	2.364	-1.621	0.735
C	2.882	-2.307	-1.519
C	1.486	-2.710	-1.138
C	1.180	-2.323	0.104
O	1.351	0.529	0.222
C	1.056	1.830	0.491
C	0.045	2.367	-0.474
O	1.567	2.444	1.410
C	0.092	3.650	-0.878

C	1.070	4.725	-0.511
C	-1.030	1.410	-0.942
C	-2.063	1.092	0.178
C	-0.090	-2.647	0.826
O	-1.037	-1.530	0.845
C	-1.812	-1.397	-0.237
C	-2.804	-0.236	-0.117
O	-1.798	-2.139	-1.203
C	-3.015	2.278	0.386
O	-3.499	-0.138	-1.357
C	-3.849	-0.640	0.970
O	-5.060	0.060	0.802
H	2.667	-2.155	1.653
H	1.884	4.361	0.113
H	1.476	5.190	-1.417
H	0.556	5.522	0.042
H	-3.616	2.450	-0.513
H	-3.703	2.111	1.216
H	-2.437	3.184	0.588
H	4.343	-0.004	1.701
H	3.805	1.419	0.800
H	5.181	-0.519	-0.533
H	3.731	0.149	-1.301
H	3.475	-3.172	-1.856
H	2.876	-1.592	-2.361
H	-0.553	0.490	-1.292
H	-1.560	1.837	-1.798
H	0.090	-2.846	1.885
H	-0.587	-3.504	0.370
H	-3.462	-0.423	1.970
H	-4.016	-1.729	0.906
H	1.944	0.044	2.147
H	-1.514	0.920	1.112
H	0.822	-3.255	-1.800
H	-0.678	3.954	-1.588
H	-3.244	-0.928	-1.866
H	-5.203	0.080	-0.159

Conformer 3

C	2.233	-0.123	1.158
C	3.683	0.343	0.969
C	4.111	-0.376	-0.317
N	3.434	-1.676	-0.244
C	2.343	-1.612	0.760
C	2.920	-2.243	-1.496
C	1.524	-2.677	-1.153
C	1.186	-2.322	0.091
O	1.341	0.537	0.227
C	1.053	1.845	0.476
C	0.060	2.376	-0.510
O	1.549	2.465	1.397
C	0.130	3.647	-0.946
C	1.127	4.711	-0.601
C	-1.030	1.423	-0.952
C	-2.018	1.098	0.203
C	-0.086	-2.700	0.781
O	-1.048	-1.595	0.861
C	-1.802	-1.387	-0.237
C	-2.785	-0.221	-0.076
O	-1.752	-2.072	-1.241
C	-2.979	2.267	0.452
O	-3.533	-0.122	-1.275
C	-3.788	-0.579	1.058
O	-3.260	-0.475	2.365
H	2.629	-2.152	1.681
H	1.926	4.347	0.044
H	1.556	5.137	-1.516
H	0.627	5.537	-0.078
H	-3.691	2.365	-0.374
H	-3.536	2.134	1.383
H	-2.418	3.203	0.534
H	4.274	-0.011	1.821
H	3.772	1.428	0.925
H	5.200	-0.489	-0.386

```

H   3.783  0.197 -1.200
H   3.531 -3.089 -1.849
H   2.918 -1.501 -2.315
H   -0.566 0.505 -1.326
H   -1.589 1.857 -1.787
H    0.088 -2.961 1.827
H   -0.571 -3.532 0.270
H   -4.198 -1.580 0.851
H   -4.618 0.127 0.989
H    1.856 0.037 2.171
H   -1.443 0.930 1.119
H    0.883 -3.219 -1.840
H   -0.633 3.948 -1.664
H   -3.210 -0.829 -1.857
H   -2.470 -1.032 2.401

```

GIAO Chemical Shielding Tensors of Retorsine

Conformer 1

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 118.2971 Anisotropy = 35.4300

XX= 128.8877 YX= -4.3810 ZX= 9.1550

XY= -8.1191 YY= 120.7654 ZY= -16.8622

XZ= 13.1827 YZ= -16.7873 ZZ= 105.2382

Eigenvalues: 93.3401 119.6340 141.9171

2 C Isotropic = 160.0854 Anisotropy = 29.8468

XX= 171.9743 YX= 13.6094 ZX= -10.9528

XY= 9.3159 YY= 154.7588 ZY= 5.7070

XZ= -13.8194 YZ= 13.6960 ZZ= 153.5230

Eigenvalues: 136.4114 163.8614 179.9832

3 C Isotropic = 143.1101 Anisotropy = 60.7200

XX= 131.3560 YX= 26.3673 ZX= 4.7023

XY= 26.3498 YY= 169.4999 ZY= 3.9217

XZ= -3.3666 YZ= 8.5922 ZZ= 128.4744

Eigenvalues: 117.4121 128.3281 183.5901

4 N Isotropic = 209.3943 Anisotropy = 68.4081

XX= 210.6918 YX= 54.9610 ZX= -31.7449

XY= 49.1303 YY= 189.3655 ZY= 32.7465

XZ= -36.6052 YZ= 44.4971 ZZ= 228.1257

Eigenvalues: 121.8978 251.2855 254.9997

5 C Isotropic = 116.7926 Anisotropy = 44.5595

XX= 138.2314 YX= 4.9414 ZX= -18.3505

XY= 12.7920 YY= 106.8557 ZY= 15.0610

XZ= -17.7027 YZ= 8.4596 ZZ= 105.2907

Eigenvalues: 86.9275 116.9514 146.4990

6 C Isotropic = 133.1322 Anisotropy = 54.4698

XX= 127.1804 YX= 16.8285 ZX= 20.2505

XY= 19.2152 YY= 125.6598 ZY= 11.8360

XZ= 18.3803 YZ= 16.7535 ZZ= 146.5565

Eigenvalues: 107.9782 121.9730 169.4454

7 C Isotropic = 56.7599 Anisotropy = 122.1683

XX= -3.8471 YX= -61.1908 ZX= -9.5190

XY= -61.7554 YY= 95.1731 ZY= -46.2646

XZ= 9.7357 YZ= -16.0435 ZZ= 78.9536

Eigenvalues: -34.9057 66.9799 138.2054

8 C Isotropic = 65.6832 Anisotropy = 125.4314

XX= 8.2118 YX= -65.1668 ZX= 2.5891

XY= -76.0752 YY= 109.5721 ZY= -11.5871

XZ= -21.2852 YZ= -32.6616 ZZ= 79.2659

Eigenvalues: -31.1427 78.8882 149.3042

9 O Isotropic = 127.7801 Anisotropy = 127.2130

XX= 130.0498 YX= 38.2442 ZX= -90.7903

XY= -34.3119 YY= 212.2565 ZY= -55.0787

XZ= -143.5551 YZ= 58.2208 ZZ= 41.0340

Eigenvalues: -39.8222 210.5738 212.5888

10 C Isotropic = 32.7746 Anisotropy = 81.3721

XX= 49.0285 YX= 44.3055 ZX= -29.3964

XY= 65.6309 YY= -15.2297 ZY= 29.3188

XZ= -14.9342 YZ= 5.3260 ZZ= 64.5251

Eigenvalues: -52.6081 63.9093 87.0227

11 C Isotropic = 63.7546 Anisotropy = 119.2960
 XX= 32.1379 YX= -25.4996 ZX= -79.4651
 XY= -26.0448 YY= 80.4041 ZY= 4.9857
 XZ= -73.0142 YZ= 12.5024 ZZ= 78.7218
 Eigenvalues: -26.6044 74.5829 143.2853
 12 O Isotropic = -79.1781 Anisotropy = 584.1643
 XX= 89.5452 YX= 94.7760 ZX= -228.4047
 XY= 102.2926 YY= -214.6684 ZY= -131.7300
 XZ= -262.3055 YZ= -186.2744 ZZ= -112.4111
 Eigenvalues: -347.4206 -200.3784 310.2648
 13 C Isotropic = 57.9259 Anisotropy = 146.7471
 XX= 30.5599 YX= -17.9664 ZX= -93.3368
 XY= -16.8519 YY= 68.6785 ZY= 26.4992
 XZ= -89.1304 YZ= 18.7650 ZZ= 74.5393
 Eigenvalues: -41.2977 59.3180 155.7573
 14 C Isotropic = 178.9569 Anisotropy = 22.8550
 XX= 186.9880 YX= 13.4017 ZX= -3.8940
 XY= 9.4725 YY= 176.0073 ZY= 8.2432
 XZ= -3.8746 YZ= 5.6287 ZZ= 173.8755
 Eigenvalues: 163.0082 179.6690 194.1936
 15 C Isotropic = 156.6956 Anisotropy = 20.7363
 XX= 165.1452 YX= 8.3580 ZX= -1.5766
 XY= 9.5430 YY= 155.3537 ZY= -0.8278
 XZ= -1.2726 YZ= 0.9439 ZZ= 149.5879
 Eigenvalues: 148.9647 150.6024 170.5198
 16 C Isotropic = 156.6988 Anisotropy = 24.6846
 XX= 161.4541 YX= 11.9949 ZX= 1.8705
 XY= 13.3433 YY= 159.2161 ZY= 3.0310
 XZ= 3.0429 YZ= -3.8115 ZZ= 149.4262
 Eigenvalues: 146.3483 150.5929 173.1552
 17 C Isotropic = 133.2269 Anisotropy = 54.6546
 XX= 143.8274 YX= -25.0471 ZX= -10.0829
 XY= -22.0258 YY= 147.9441 ZY= -10.2510
 XZ= -6.3037 YZ= -12.7796 ZZ= 107.9093
 Eigenvalues: 99.4214 130.5961 169.6633
 18 O Isotropic = 145.1475 Anisotropy = 165.0444
 XX= 192.1643 YX= 69.1155 ZX= -23.9530
 XY= 114.6272 YY= 95.0373 ZY= -33.4664
 XZ= 79.3026 YZ= -146.8844 ZZ= 148.2409
 Eigenvalues: -12.9379 193.2033 255.1771
 19 C Isotropic = 21.1367 Anisotropy = 97.1355
 XX= 9.6210 YX= 62.5983 ZX= -38.3997
 XY= 46.7472 YY= 39.5511 ZY= 10.0446
 XZ= -59.1471 YZ= 25.8512 ZZ= 14.2378
 Eigenvalues: -64.2006 41.7169 85.8936
 20 C Isotropic = 111.9023 Anisotropy = 17.1007
 XX= 117.6620 YX= 5.4673 ZX= 11.6103
 XY= 7.6885 YY= 111.3355 ZY= -10.6250
 XZ= 7.2451 YZ= -15.1541 ZZ= 106.7094
 Eigenvalues: 91.0019 121.4022 123.3027
 21 O Isotropic = -47.8528 Anisotropy = 591.1316
 XX= 59.4301 YX= 222.8414 ZX= -157.8662
 XY= 211.9019 YY= 44.2697 ZY= -133.0928
 XZ= -187.6291 YZ= -123.3599 ZZ= -247.2581
 Eigenvalues: -328.1711 -161.6221 346.2349
 22 C Isotropic = 182.4629 Anisotropy = 19.4339
 XX= 184.6538 YX= -9.5407 ZX= -4.6308
 XY= -12.1680 YY= 183.1809 ZY= 1.0903
 XZ= -4.4184 YZ= -1.7143 ZZ= 179.5541
 Eigenvalues: 171.5825 180.3874 195.4189
 23 O Isotropic = 307.1129 Anisotropy = 62.0687
 XX= 305.6724 YX= -39.6522 ZX= -4.5172
 XY= -40.3214 YY= 297.1139 ZY= 3.0364
 XZ= -9.5672 YZ= 24.0106 ZZ= 318.5525
 Eigenvalues: 260.6609 312.1858 348.4921
 24 C Isotropic = 129.7327 Anisotropy = 41.1517
 XX= 128.7513 YX= 21.9627 ZX= -4.8273
 XY= 18.7411 YY= 142.5278 ZY= 1.6607
 XZ= -1.4140 YZ= 5.9407 ZZ= 117.9190
 Eigenvalues: 110.9148 121.1161 157.1672
 25 O Isotropic = 318.5106 Anisotropy = 43.1688
 XX= 293.9088 YX= -24.8363 ZX= -3.1320
 XY= 6.0107 YY= 314.4310 ZY= -6.0603
 XZ= 7.4428 YZ= 5.6579 ZZ= 347.1919

Eigenvalues: 290.1797 318.0623 347.2898
 26 H Isotropic = 27.4326 Anisotropy = 7.3912
 XX= 25.8409 YX= -0.1994 ZX= 0.1842
 XY= -0.5248 YY= 26.7574 ZY= -3.5170
 XZ= -0.3177 YZ= -4.1971 ZZ= 29.6997
 Eigenvalues: 24.0377 25.9001 32.3601
 27 H Isotropic = 28.9206 Anisotropy = 6.1901
 XX= 28.7809 YX= 0.2834 ZX= 4.3255
 XY= 1.2030 YY= 30.7099 ZY= -1.9655
 XZ= 3.5760 YZ= -3.7360 ZZ= 27.2709
 Eigenvalues: 23.0512 30.6633 33.0473
 28 H Isotropic = 30.3452 Anisotropy = 9.9574
 XX= 29.2209 YX= 3.7828 ZX= -3.7468
 XY= 2.6346 YY= 30.3746 ZY= -3.3049
 XZ= -2.4484 YZ= -3.6743 ZZ= 31.4401
 Eigenvalues: 26.5257 27.5265 36.9835
 29 H Isotropic = 30.0065 Anisotropy = 9.6755
 XX= 27.7899 YX= -1.2312 ZX= -0.8309
 XY= -1.6802 YY= 34.9670 ZY= 2.8855
 XZ= -1.1556 YZ= 3.5063 ZZ= 27.2626
 Eigenvalues: 25.9820 27.5806 36.4568
 30 H Isotropic = 30.8014 Anisotropy = 8.7591
 XX= 32.6088 YX= -2.5889 ZX= 4.0206
 XY= -3.3539 YY= 30.7253 ZY= -1.3191
 XZ= 3.7964 YZ= -0.4276 ZZ= 29.0701
 Eigenvalues: 26.3231 29.4403 36.6408
 31 H Isotropic = 31.0668 Anisotropy = 10.5702
 XX= 30.4877 YX= -0.9308 ZX= -5.8803
 XY= -2.0244 YY= 30.0950 ZY= 2.0915
 XZ= -5.7464 YZ= 1.3932 ZZ= 32.6177
 Eigenvalues: 25.6425 29.4443 38.1136
 32 H Isotropic = 30.7093 Anisotropy = 8.4979
 XX= 31.0901 YX= 1.6673 ZX= -1.3754
 XY= 1.9322 YY= 35.6413 ZY= 1.7889
 XZ= -2.2208 YZ= 1.6691 ZZ= 25.3965
 Eigenvalues: 24.4506 31.3028 36.3745
 33 H Isotropic = 29.8527 Anisotropy = 10.7498
 XX= 31.9706 YX= -0.1168 ZX= 5.1663
 XY= -0.7271 YY= 25.5523 ZY= 0.4959
 XZ= 4.8420 YZ= 1.3872 ZZ= 32.0352
 Eigenvalues: 25.0620 27.4769 37.0192
 34 H Isotropic = 29.0516 Anisotropy = 8.6617
 XX= 29.5351 YX= 1.3771 ZX= 0.9215
 XY= 1.1464 YY= 34.0729 ZY= 2.3774
 XZ= -0.7139 YZ= 2.0898 ZZ= 23.5467
 Eigenvalues: 23.0888 29.2399 34.8260
 35 H Isotropic = 28.6371 Anisotropy = 11.0472
 XX= 35.5824 YX= 0.3968 ZX= -2.0556
 XY= 2.3836 YY= 26.0296 ZY= 0.7912
 XZ= -1.4169 YZ= 0.8675 ZZ= 24.2993
 Eigenvalues: 23.5834 26.3260 36.0019
 36 H Isotropic = 29.2178 Anisotropy = 6.7846
 XX= 27.4620 YX= 0.5461 ZX= -1.7716
 XY= 0.9455 YY= 29.9447 ZY= -3.8165
 XZ= -2.5735 YZ= -2.0448 ZZ= 30.2467
 Eigenvalues: 26.0310 27.8816 33.7409
 37 H Isotropic = 27.7868 Anisotropy = 10.7887
 XX= 26.7203 YX= -2.1366 ZX= -1.4189
 XY= -3.6322 YY= 28.9633 ZY= 5.3876
 XZ= -1.6083 YZ= 5.4187 ZZ= 27.6768
 Eigenvalues: 22.6830 25.6982 34.9792
 38 H Isotropic = 28.3701 Anisotropy = 7.0221
 XX= 26.3535 YX= -0.7453 ZX= -0.0111
 XY= 1.3738 YY= 25.7733 ZY= 0.0682
 XZ= -1.3352 YZ= -0.1116 ZZ= 32.9834
 Eigenvalues: 25.6267 26.4321 33.0515
 39 H Isotropic = 29.3345 Anisotropy = 5.2458
 XX= 30.7822 YX= -0.9214 ZX= -0.8953
 XY= -1.5080 YY= 31.7184 ZY= 0.6418
 XZ= -0.8913 YZ= 1.6040 ZZ= 25.5029
 Eigenvalues: 25.2213 29.9505 32.8317
 40 H Isotropic = 30.1175 Anisotropy = 5.4567
 XX= 29.0819 YX= 1.2528 ZX= 1.2471
 XY= 1.5645 YY= 29.2917 ZY= -2.4531

XZ= 1.3391 YZ= -3.1137 ZZ= 31.9790
 Eigenvalues: 26.2767 30.3206 33.7553
 41 H Isotropic = 27.6312 Anisotropy = 7.1965
 XX= 27.0602 YX= -1.0955 ZX= -0.0138
 XY= -1.3818 YY= 27.1075 ZY= -5.4016
 XZ= -0.2040 YZ= -3.2823 ZZ= 28.7260
 Eigenvalues: 23.2236 27.2412 32.4288
 42 H Isotropic = 26.1401 Anisotropy = 6.0424
 XX= 26.2640 YX= -0.2042 ZX= -0.5374
 XY= 0.4146 YY= 30.1643 ZY= 1.2232
 XZ= -0.4419 YZ= -1.0036 ZZ= 21.9919
 Eigenvalues: 21.9348 26.3172 30.1683
 43 H Isotropic = 27.9522 Anisotropy = 6.4638
 XX= 28.3437 YX= 1.0286 ZX= -3.2072
 XY= -0.0796 YY= 31.8723 ZY= 1.7325
 XZ= -3.6468 YZ= 1.8288 ZZ= 23.6405
 Eigenvalues: 21.5234 30.0717 32.2614
 44 H Isotropic = 28.0707 Anisotropy = 2.7206
 XX= 27.7599 YX= 1.1321 ZX= 0.3312
 XY= 2.0490 YY= 26.5927 ZY= -0.0970
 XZ= -0.0438 YZ= -0.4754 ZZ= 29.8596
 Eigenvalues: 25.4592 28.8685 29.8845
 45 H Isotropic = 26.9790 Anisotropy = 3.9103
 XX= 26.6164 YX= -0.6763 ZX= 0.0121
 XY= -0.8427 YY= 24.9036 ZY= -1.4197
 XZ= -0.5692 YZ= -0.3239 ZZ= 29.4169
 Eigenvalues: 24.4472 26.9038 29.5859
 46 H Isotropic = 30.0850 Anisotropy = 5.7304
 XX= 32.1494 YX= -0.8587 ZX= 2.9021
 XY= -0.6938 YY= 28.9185 ZY= -0.0492
 XZ= 2.1272 YZ= -2.2822 ZZ= 29.1871
 Eigenvalues: 27.4310 28.9187 33.9053
 47 H Isotropic = 25.0793 Anisotropy = 4.5864
 XX= 25.1002 YX= -2.0285 ZX= -2.8323
 XY= -1.0981 YY= 23.7421 ZY= 0.1784
 XZ= 0.6535 YZ= 3.1037 ZZ= 26.3956
 Eigenvalues: 22.5148 24.5862 28.1369
 48 H Isotropic = 25.6546 Anisotropy = 8.0779
 XX= 24.2297 YX= 3.0571 ZX= -0.7005
 XY= 2.8270 YY= 29.3166 ZY= -1.3486
 XZ= -0.4442 YZ= -1.8585 ZZ= 23.4174
 Eigenvalues: 22.7991 23.1248 31.0399
 49 H Isotropic = 28.2712 Anisotropy = 19.3048
 XX= 25.4550 YX= -6.4159 ZX= -2.7531
 XY= -6.5927 YY= 28.0821 ZY= 8.3592
 XZ= -2.6760 YZ= 9.1227 ZZ= 31.2766
 Eigenvalues: 18.6188 25.0538 41.1411
 50 H Isotropic = 30.3778 Anisotropy = 14.9387
 XX= 29.2028 YX= 5.8264 ZX= 6.1579
 XY= 4.4445 YY= 24.7521 ZY= -1.2733
 XZ= 5.6466 YZ= -2.9193 ZZ= 37.1785
 Eigenvalues: 19.8436 30.9529 40.3369

Conformer 2

1 C Isotropic = 118.8594 Anisotropy = 35.2074
 XX= 130.6916 YX= -4.7833 ZX= 8.2567
 XY= -8.5825 YY= 121.2657 ZY= -16.5420
 XZ= 11.9145 YZ= -16.5582 ZZ= 104.6208
 Eigenvalues: 93.6564 120.5908 142.3310
 2 C Isotropic = 160.0414 Anisotropy = 29.4846
 XX= 170.7418 YX= 13.6603 ZX= -11.6768
 XY= 8.9537 YY= 155.3641 ZY= 4.8087
 XZ= -14.8102 YZ= 12.9699 ZZ= 154.0183
 Eigenvalues: 136.8415 163.5849 179.6978
 3 C Isotropic = 142.9119 Anisotropy = 60.7144
 XX= 130.6802 YX= 26.7596 ZX= 4.2607
 XY= 26.5195 YY= 169.5664 ZY= 2.1789
 XZ= -4.7645 YZ= 6.9379 ZZ= 128.4891
 Eigenvalues: 116.6897 128.6578 183.3882
 4 N Isotropic = 209.6960 Anisotropy = 67.6410
 XX= 208.1492 YX= 54.7160 ZX= -32.3123
 XY= 48.5990 YY= 191.9383 ZY= 32.6903
 XZ= -37.0497 YZ= 43.9475 ZZ= 229.0005
 Eigenvalues: 122.6532 251.6448 254.7900

5 C Isotropic = 116.6724 Anisotropy = 45.3038
 XX= 137.5352 YX= 5.0184 ZX= -19.6552
 XY= 12.3234 YY= 106.4946 ZY= 15.0144
 XZ= -18.9483 YZ= 9.4646 ZZ= 105.9875
 Eigenvalues: 86.0821 117.0601 146.8749

6 C Isotropic = 133.2056 Anisotropy = 54.4252
 XX= 128.7701 YX= 17.7976 ZX= 20.0731
 XY= 19.4105 YY= 126.1290 ZY= 12.3530
 XZ= 18.5875 YZ= 16.6153 ZZ= 144.7177
 Eigenvalues: 108.4809 121.6469 169.4890

7 C Isotropic = 56.6010 Anisotropy = 122.6951
 XX= -6.1856 YX= -60.5974 ZX= -7.0676
 XY= -59.7375 YY= 96.3436 ZY= -45.4914
 XZ= 12.5189 YZ= -15.4494 ZZ= 79.6451
 Eigenvalues: -34.9362 66.3415 138.3978

8 C Isotropic = 65.4763 Anisotropy = 125.6448
 XX= 4.8773 YX= -63.5870 ZX= 5.5089
 XY= -75.3029 YY= 110.8925 ZY= -10.6153
 XZ= -17.9031 YZ= -32.0905 ZZ= 80.6591
 Eigenvalues: -31.5183 78.7077 149.2395

9 O Isotropic = 127.8892 Anisotropy = 128.1077
 XX= 123.3972 YX= 40.3025 ZX= -91.2884
 XY= -34.3894 YY= 212.9762 ZY= -51.1552
 XZ= -145.9159 YZ= 56.0550 ZZ= 47.2941
 Eigenvalues: -39.2660 209.6392 213.2943

10 C Isotropic = 32.8605 Anisotropy = 80.9091
 XX= 47.8476 YX= 44.4676 ZX= -28.0970
 XY= 66.4994 YY= -15.7500 ZY= 26.3399
 XZ= -13.3548 YZ= 3.1438 ZZ= 66.4837
 Eigenvalues: -52.4382 64.2197 86.7999

11 C Isotropic = 64.2462 Anisotropy = 119.8926
 XX= 33.0840 YX= -23.5184 ZX= -80.4378
 XY= -24.1947 YY= 78.7925 ZY= 3.6902
 XZ= -73.9459 YZ= 11.4479 ZZ= 80.8621
 Eigenvalues: -25.9473 74.5113 144.1746

12 O Isotropic = -77.5665 Anisotropy = 582.9867
 XX= 75.1112 YX= 91.5048 ZX= -233.0669
 XY= 101.5533 YY= -208.1002 ZY= -136.9978
 XZ= -266.8039 YZ= -187.9726 ZZ= -99.7105
 Eigenvalues: -344.8050 -198.9858 311.0913

13 C Isotropic = 56.7479 Anisotropy = 148.4275
 XX= 28.8216 YX= -16.9946 ZX= -94.3489
 XY= -14.8076 YY= 64.7743 ZY= 24.5862
 XZ= -89.9864 YZ= 17.9156 ZZ= 76.6478
 Eigenvalues: -42.4863 57.0305 155.6996

14 C Isotropic = 178.7488 Anisotropy = 23.0864
 XX= 186.2368 YX= 14.0276 ZX= -3.7861
 XY= 10.0923 YY= 175.7273 ZY= 7.8619
 XZ= -4.1798 YZ= 5.0863 ZZ= 174.2823
 Eigenvalues: 162.7990 179.3077 194.1397

15 C Isotropic = 155.6322 Anisotropy = 21.2630
 XX= 164.5700 YX= 8.8664 ZX= -2.2023
 XY= 9.3398 YY= 153.5687 ZY= 0.3526
 XZ= -1.6019 YZ= 0.4293 ZZ= 148.7579
 Eigenvalues: 147.2676 149.8213 169.8075

16 C Isotropic = 153.5745 Anisotropy = 28.5469
 XX= 157.1999 YX= 15.0925 ZX= 2.7049
 XY= 18.1820 YY= 154.4839 ZY= 1.9844
 XZ= 1.9976 YZ= -3.2723 ZZ= 149.0396
 Eigenvalues: 138.7328 149.3849 172.6058

17 C Isotropic = 133.6778 Anisotropy = 55.0343
 XX= 143.6852 YX= -25.9272 ZX= -9.9338
 XY= -22.6847 YY= 147.3987 ZY= -13.3581
 XZ= -5.8852 YZ= -14.9142 ZZ= 109.9495
 Eigenvalues: 98.9226 131.7435 170.3674

18 O Isotropic = 140.7118 Anisotropy = 165.7172
 XX= 190.7615 YX= 59.7338 ZX= -34.1211
 XY= 112.4143 YY= 74.3456 ZY= -35.3791
 XZ= 60.6729 YZ= -143.1421 ZZ= 157.0284
 Eigenvalues: -14.4583 185.4039 251.1899

19 C Isotropic = 21.3655 Anisotropy = 97.2251
 XX= 8.9162 YX= 60.0065 ZX= -43.3441
 XY= 43.2360 YY= 42.3201 ZY= 10.1046
 XZ= -61.9964 YZ= 22.8157 ZZ= 12.8603

Eigenvalues: -64.8215 42.7359 86.1823
 20 C Isotropic = 115.0263 Anisotropy = 24.8418
 XX= 122.5894 YX= 7.7244 ZX= 12.3419
 XY= 0.9042 YY= 107.8566 ZY= -13.6087
 XZ= 11.8320 YZ= -5.8720 ZZ= 114.6329
 Eigenvalues: 96.3411 117.1503 131.5875
 21 O Isotropic = -31.2560 Anisotropy = 567.2190
 XX= 65.3756 YX= 216.5989 ZX= -154.7336
 XY= 183.7761 YY= 26.1918 ZY= -141.4158
 XZ= -206.5636 YZ= -146.6200 ZZ= -185.3353
 Eigenvalues: -286.6123 -154.0456 346.8900
 22 C Isotropic = 181.7310 Anisotropy = 16.7729
 XX= 184.0981 YX= -8.8261 ZX= -2.8921
 XY= -10.1803 YY= 181.1498 ZY= 2.4376
 XZ= -4.7856 YZ= -2.4339 ZZ= 179.9450
 Eigenvalues: 172.1605 180.1196 192.9129
 23 O Isotropic = 310.5067 Anisotropy = 76.9418
 XX= 283.3327 YX= -15.7362 ZX= -4.8592
 XY= -16.0262 YY= 328.5821 ZY= 42.2528
 XZ= 6.3064 YZ= 29.1987 ZZ= 319.6053
 Eigenvalues: 273.4716 296.2473 361.8012
 24 C Isotropic = 129.6556 Anisotropy = 41.8397
 XX= 152.1438 YX= -15.3226 ZX= -5.8476
 XY= -12.3314 YY= 121.8397 ZY= -3.3922
 XZ= 3.0362 YZ= -11.3362 ZZ= 114.9832
 Eigenvalues: 108.2985 123.1195 157.5487
 25 O Isotropic = 316.3618 Anisotropy = 57.3266
 XX= 288.3031 YX= 12.2969 ZX= -14.7501
 XY= -17.0231 YY= 308.3854 ZY= -5.4280
 XZ= -4.7890 YZ= -6.9711 ZZ= 352.3970
 Eigenvalues: 286.3562 308.1498 354.5795
 26 H Isotropic = 27.4334 Anisotropy = 7.3682
 XX= 25.7796 YX= -0.3148 ZX= 0.2437
 XY= -0.6956 YY= 26.6791 ZY= -3.4488
 XZ= -0.1784 YZ= -4.0536 ZZ= 29.8415
 Eigenvalues: 24.0926 25.8621 32.3455
 27 H Isotropic = 28.8939 Anisotropy = 6.1716
 XX= 29.1306 YX= -0.0038 ZX= 4.3042
 XY= 0.9499 YY= 30.8547 ZY= -1.7789
 XZ= 3.5890 YZ= -3.5705 ZZ= 26.6965
 Eigenvalues: 23.0129 30.6606 33.0083
 28 H Isotropic = 30.3476 Anisotropy = 9.9624
 XX= 28.8123 YX= 3.8975 ZX= -3.2652
 XY= 2.6039 YY= 30.9417 ZY= -3.5894
 XZ= -1.9654 YZ= -3.9498 ZZ= 31.2889
 Eigenvalues: 26.4513 27.6023 36.9892
 29 H Isotropic = 29.9486 Anisotropy = 9.5901
 XX= 27.7513 YX= -1.2495 ZX= -1.0725
 XY= -1.6293 YY= 34.3669 ZY= 3.3444
 XZ= -1.4002 YZ= 3.8906 ZZ= 27.7274
 Eigenvalues: 25.9324 27.5713 36.3420
 30 H Isotropic = 30.9261 Anisotropy = 8.0386
 XX= 31.8372 YX= -2.3219 ZX= 3.8474
 XY= -2.6429 YY= 31.3746 ZY= -1.9534
 XZ= 3.3799 YZ= -1.3166 ZZ= 29.5666
 Eigenvalues: 26.9072 29.5860 36.2852
 31 H Isotropic = 30.1069 Anisotropy = 9.6809
 XX= 30.9919 YX= 0.2389 ZX= -5.7798
 XY= -0.3324 YY= 29.4270 ZY= 2.0198
 XZ= -6.0565 YZ= 1.1292 ZZ= 29.9018
 Eigenvalues: 24.2513 29.5085 36.5608
 32 H Isotropic = 30.6848 Anisotropy = 8.7177
 XX= 31.1493 YX= 1.8459 ZX= -0.7625
 XY= 2.0513 YY= 35.2743 ZY= 2.8905
 XZ= -1.7351 YZ= 2.6745 ZZ= 25.6310
 Eigenvalues: 24.4359 31.1220 36.4967
 33 H Isotropic = 29.8454 Anisotropy = 10.7684
 XX= 32.4039 YX= 0.0007 ZX= 5.1889
 XY= -0.6988 YY= 25.5774 ZY= 0.6309
 XZ= 4.8264 YZ= 1.5151 ZZ= 31.5547
 Eigenvalues: 25.0156 27.4962 37.0243
 34 H Isotropic = 29.1431 Anisotropy = 8.6641
 XX= 29.6090 YX= 1.5200 ZX= 0.5830
 XY= 1.2671 YY= 34.1934 ZY= 2.2366

XZ= -0.9933 YZ= 1.9026 ZZ= 23.6270
 Eigenvalues: 23.2023 29.3080 34.9192
 35 H Isotropic = 28.6668 Anisotropy = 11.0013
 XX= 35.3604 YX= 0.4709 ZX= -2.5937
 XY= 2.4749 YY= 26.1269 ZY= 0.6550
 XZ= -2.0155 YZ= 0.8325 ZZ= 24.5131
 Eigenvalues: 23.6052 26.3942 36.0010
 36 H Isotropic = 29.2382 Anisotropy = 6.6608
 XX= 27.3187 YX= 0.3815 ZX= -1.5990
 XY= 0.6817 YY= 29.8787 ZY= -3.8012
 XZ= -2.3481 YZ= -2.0570 ZZ= 30.5171
 Eigenvalues: 26.1047 27.9312 33.6787
 37 H Isotropic = 27.7838 Anisotropy = 10.7950
 XX= 26.6089 YX= -2.0140 ZX= -1.2800
 XY= -3.5353 YY= 29.3818 ZY= 5.4737
 XZ= -1.3934 YZ= 5.4139 ZZ= 27.3606
 Eigenvalues: 22.6581 25.7128 34.9805
 38 H Isotropic = 28.3588 Anisotropy = 7.1180
 XX= 26.3177 YX= -0.6284 ZX= 0.1297
 XY= 1.4363 YY= 25.7015 ZY= 0.2816
 XZ= -1.2076 YZ= 0.1336 ZZ= 33.0571
 Eigenvalues: 25.4772 26.4950 33.1041
 39 H Isotropic = 29.3353 Anisotropy = 5.3905
 XX= 31.2633 YX= -1.1368 ZX= -0.7073
 XY= -1.7580 YY= 31.2920 ZY= 0.6532
 XZ= -0.6731 YZ= 1.4499 ZZ= 25.4505
 Eigenvalues: 25.2340 29.8428 32.9289
 40 H Isotropic = 29.9509 Anisotropy = 5.2377
 XX= 28.9253 YX= 1.3837 ZX= 0.9945
 XY= 1.8029 YY= 29.1044 ZY= -2.2209
 XZ= 1.3953 YZ= -3.0595 ZZ= 31.8230
 Eigenvalues: 26.1004 30.3096 33.4427
 41 H Isotropic = 27.7744 Anisotropy = 7.1141
 XX= 27.1279 YX= -1.0169 ZX= -0.0646
 XY= -1.4137 YY= 26.8910 ZY= -5.2446
 XZ= -0.0446 YZ= -3.0727 ZZ= 29.3045
 Eigenvalues: 23.4864 27.3198 32.5172
 42 H Isotropic = 26.2155 Anisotropy = 6.0199
 XX= 26.2019 YX= -0.2481 ZX= -0.5242
 XY= 0.6433 YY= 30.2033 ZY= 0.8361
 XZ= -0.3880 YZ= -1.4971 ZZ= 22.2413
 Eigenvalues: 22.1777 26.2400 30.2287
 43 H Isotropic = 28.0530 Anisotropy = 3.6097
 XX= 29.1463 YX= -0.9105 ZX= 0.7021
 XY= -0.8383 YY= 25.1233 ZY= -1.7089
 XZ= -0.3766 YZ= -1.3081 ZZ= 29.8893
 Eigenvalues: 24.5479 29.1516 30.4594
 44 H Isotropic = 28.4317 Anisotropy = 6.3118
 XX= 30.1855 YX= -1.9573 ZX= -1.8461
 XY= 0.3504 YY= 31.9469 ZY= -2.4366
 XZ= -2.1894 YZ= -2.5500 ZZ= 23.1627
 Eigenvalues: 21.9402 30.7154 32.6396
 45 H Isotropic = 26.9489 Anisotropy = 3.9481
 XX= 26.3948 YX= -0.6868 ZX= 0.1376
 XY= -1.0607 YY= 24.9833 ZY= -1.2505
 XZ= -0.4406 YZ= -0.1868 ZZ= 29.4685
 Eigenvalues: 24.4638 26.8019 29.5809
 46 H Isotropic = 29.9040 Anisotropy = 5.8897
 XX= 31.9068 YX= -0.8021 ZX= 2.9426
 XY= -1.3709 YY= 28.6462 ZY= 0.1058
 XZ= 2.1297 YZ= -2.1680 ZZ= 29.1590
 Eigenvalues: 27.5084 28.3731 33.8305
 47 H Isotropic = 25.1042 Anisotropy = 4.6665
 XX= 25.0567 YX= -2.0560 ZX= -2.8159
 XY= -1.0547 YY= 23.9301 ZY= 0.3886
 XZ= 0.7014 YZ= 3.2193 ZZ= 26.3260
 Eigenvalues: 22.5643 24.5331 28.2153
 48 H Isotropic = 25.5820 Anisotropy = 8.3078
 XX= 24.0931 YX= 3.1933 ZX= -0.6931
 XY= 2.8594 YY= 29.4470 ZY= -1.1690
 XZ= -0.3986 YZ= -1.7756 ZZ= 23.2059
 Eigenvalues: 22.6788 22.9467 31.1206
 49 H Isotropic = 28.5747 Anisotropy = 20.6837
 XX= 23.7038 YX= -4.8907 ZX= 1.3595

XY= -5.5497 YY= 33.3387 ZY= 10.4216
 XZ= 0.0967 YZ= 10.3119 ZZ= 28.6816
 Eigenvalues: 17.6975 25.6628 42.3638
 50 H Isotropic = 29.6811 Anisotropy = 14.3756
 XX= 31.0769 YX= -2.5160 ZX= 1.9452
 XY= -0.1595 YY= 19.0805 ZY= -0.7469
 XZ= 1.5154 YZ= 0.2861 ZZ= 38.8860
 Eigenvalues: 18.9331 30.8455 39.2649

Conformer 3

1 C Isotropic = 118.5093 Anisotropy = 34.9059
 XX= 129.2366 YX= -4.4025 ZX= 8.7330
 XY= -8.0950 YY= 120.8610 ZY= -16.6286
 XZ= 12.7676 YZ= -16.6233 ZZ= 105.4304
 Eigenvalues: 93.8077 119.9403 141.7799
 2 C Isotropic = 160.1555 Anisotropy = 29.6971
 XX= 171.8442 YX= 13.5787 ZX= -11.1326
 XY= 9.2688 YY= 154.8197 ZY= 5.6313
 XZ= -13.8014 YZ= 13.6007 ZZ= 153.8025
 Eigenvalues: 136.5761 163.9368 179.9535
 3 C Isotropic = 143.1046 Anisotropy = 60.7768
 XX= 131.1623 YX= 26.3192 ZX= 4.7257
 XY= 26.3719 YY= 169.6561 ZY= 3.7847
 XZ= -3.6487 YZ= 8.4095 ZZ= 128.4953
 Eigenvalues: 117.2963 128.3950 183.6225
 4 N Isotropic = 209.0476 Anisotropy = 68.5063
 XX= 210.2106 YX= 55.4629 ZX= -31.7658
 XY= 48.7709 YY= 188.9686 ZY= 32.4824
 XZ= -36.5816 YZ= 44.4280 ZZ= 227.9638
 Eigenvalues: 121.5623 250.8621 254.7185
 5 C Isotropic = 116.8525 Anisotropy = 44.2724
 XX= 138.0886 YX= 4.7984 ZX= -18.3543
 XY= 12.5998 YY= 107.0901 ZY= 14.9947
 XZ= -17.6986 YZ= 8.4153 ZZ= 105.3789
 Eigenvalues: 87.1537 117.0365 146.3675
 6 C Isotropic = 133.0753 Anisotropy = 54.1192
 XX= 127.2099 YX= 16.7443 ZX= 20.0902
 XY= 19.1617 YY= 125.8010 ZY= 11.7335
 XZ= 18.3653 YZ= 16.7005 ZZ= 146.2151
 Eigenvalues: 108.1197 121.9515 169.1548
 7 C Isotropic = 55.7005 Anisotropy = 123.8442
 XX= -4.5340 YX= -61.8636 ZX= -9.3819
 XY= -62.3788 YY= 94.1115 ZY= -47.5873
 XZ= 10.0495 YZ= -16.6291 ZZ= 77.5240
 Eigenvalues: -36.2519 65.0901 138.2633
 8 C Isotropic = 65.8620 Anisotropy = 125.3808
 XX= 8.5863 YX= -65.6005 ZX= 3.3645
 XY= -76.6048 YY= 109.3007 ZY= -10.8823
 XZ= -20.3851 YZ= -32.0505 ZZ= 79.6990
 Eigenvalues: -30.9602 79.0970 149.4492
 9 O Isotropic = 129.4930 Anisotropy = 128.5389
 XX= 128.9665 YX= 37.4143 ZX= -90.8094
 XY= -35.3546 YY= 215.0328 ZY= -53.5212
 XZ= -142.5405 YZ= 58.9929 ZZ= 44.4797
 Eigenvalues: -37.3955 210.6889 215.1856
 10 C Isotropic = 32.8522 Anisotropy = 81.0290
 XX= 49.7647 YX= 43.8273 ZX= -28.5726
 XY= 65.3831 YY= -16.5379 ZY= 28.7893
 XZ= -14.1141 YZ= 4.7964 ZZ= 65.3297
 Eigenvalues: -52.6451 64.3301 86.8715
 11 C Isotropic = 63.5951 Anisotropy = 119.5365
 XX= 31.8504 YX= -24.2747 ZX= -79.9763
 XY= -25.0275 YY= 79.9016 ZY= 4.6690
 XZ= -73.5768 YZ= 12.6598 ZZ= 79.0333
 Eigenvalues: -26.9493 74.4485 143.2861
 12 O Isotropic = -79.2794 Anisotropy = 584.3785
 XX= 86.5086 YX= 91.2297 ZX= -230.5198
 XY= 98.4667 YY= -215.3394 ZY= -131.7104
 XZ= -266.4159 YZ= -185.4716 ZZ= -109.0075
 Eigenvalues: -348.1783 -199.9662 310.3062
 13 C Isotropic = 57.8176 Anisotropy = 147.1143
 XX= 29.5453 YX= -17.6008 ZX= -93.3792
 XY= -16.1548 YY= 67.5586 ZY= 26.0298
 XZ= -89.1976 YZ= 17.9817 ZZ= 76.3489

Eigenvalues: -41.2933 58.8523 155.8938
 14 C Isotropic = 178.7625 Anisotropy = 22.8827
 XX= 186.5798 YX= 13.5839 ZX= -3.9263
 XY= 9.7216 YY= 175.7568 ZY= 7.8370
 XZ= -4.0677 YZ= 5.2506 ZZ= 173.9509
 Eigenvalues: 162.9684 179.3015 194.0176
 15 C Isotropic = 156.8566 Anisotropy = 20.8567
 XX= 165.8326 YX= 8.6952 ZX= -1.3608
 XY= 8.3020 YY= 155.8182 ZY= -0.8564
 XZ= -1.5081 YZ= 0.8351 ZZ= 148.9191
 Eigenvalues: 148.6359 151.1729 170.7611
 16 C Isotropic = 157.4223 Anisotropy = 20.6423
 XX= 162.6060 YX= 8.7894 ZX= -1.0555
 XY= 9.7146 YY= 161.1838 ZY= 3.7987
 XZ= 1.6688 YZ= -5.8352 ZZ= 148.4771
 Eigenvalues: 148.2581 152.8250 171.1838
 17 C Isotropic = 133.4183 Anisotropy = 54.9097
 XX= 145.1181 YX= -24.9435 ZX= -11.9483
 XY= -21.7200 YY= 147.9768 ZY= -11.6639
 XZ= -6.9134 YZ= -12.7452 ZZ= 107.1601
 Eigenvalues: 97.8987 132.3315 170.0248
 18 O Isotropic = 143.7082 Anisotropy = 148.7889
 XX= 188.8175 YX= 57.5370 ZX= -27.5415
 XY= 89.2714 YY= 93.0193 ZY= -45.8932
 XZ= 67.1941 YZ= -139.6701 ZZ= 149.2878
 Eigenvalues: -2.4696 190.6934 242.9008
 19 C Isotropic = 19.6907 Anisotropy = 96.5227
 XX= 9.4693 YX= 60.2394 ZX= -41.3498
 XY= 43.5176 YY= 44.0808 ZY= 19.8837
 XZ= -65.4334 YZ= 29.4443 ZZ= 5.5219
 Eigenvalues: -71.6010 46.6338 84.0391
 20 C Isotropic = 114.8746 Anisotropy = 24.7893
 XX= 119.3848 YX= 9.3086 ZX= 11.9457
 XY= 4.9495 YY= 109.2732 ZY= -11.3110
 XZ= 14.6047 YZ= -11.8599 ZZ= 115.9656
 Eigenvalues: 93.0876 120.1353 131.4008
 21 O Isotropic = -40.4290 Anisotropy = 573.4709
 XX= 68.8838 YX= 226.4479 ZX= -143.9067
 XY= 199.6592 YY= 33.3054 ZY= -125.2422
 XZ= -187.7451 YZ= -130.2173 ZZ= -223.4762
 Eigenvalues: -302.4953 -160.6766 341.8849
 22 C Isotropic = 183.7290 Anisotropy = 19.9612
 XX= 185.7622 YX= -10.6927 ZX= -3.6966
 XY= -12.9452 YY= 183.6566 ZY= 1.5162
 XZ= -3.4157 YZ= -1.4872 ZZ= 181.7683
 Eigenvalues: 172.2267 181.9238 197.0365
 23 O Isotropic = 305.2867 Anisotropy = 58.6318
 XX= 290.8429 YX= -30.6002 ZX= -5.4134
 XY= -27.6702 YY= 300.9601 ZY= 17.2013
 XZ= 0.1807 YZ= 27.1258 ZZ= 324.0571
 Eigenvalues: 263.5872 307.8983 344.3746
 24 C Isotropic = 130.7371 Anisotropy = 59.8579
 XX= 122.5445 YX= 7.7065 ZX= 10.8417
 XY= 6.2953 YY= 102.7784 ZY= -6.1348
 XZ= 15.7687 YZ= -2.1674 ZZ= 166.8885
 Eigenvalues: 99.5234 122.0456 170.6424
 25 O Isotropic = 310.7733 Anisotropy = 48.5078
 XX= 334.8131 YX= -17.4573 ZX= 0.9961
 XY= -20.1926 YY= 298.6459 ZY= 0.8276
 XZ= -10.0305 YZ= -4.1534 ZZ= 298.8608
 Eigenvalues: 289.4408 299.7672 343.1118
 26 H Isotropic = 27.4402 Anisotropy = 7.3399
 XX= 25.9120 YX= -0.2051 ZX= 0.1538
 XY= -0.5716 YY= 26.7510 ZY= -3.5336
 XZ= -0.3156 YZ= -4.1884 ZZ= 29.6575
 Eigenvalues: 24.0086 25.9785 32.3334
 27 H Isotropic = 28.9209 Anisotropy = 6.1196
 XX= 29.0482 YX= 0.1771 ZX= 4.2155
 XY= 1.0890 YY= 30.7679 ZY= -1.9650
 XZ= 3.4701 YZ= -3.7113 ZZ= 26.9465
 Eigenvalues: 23.0860 30.6760 33.0006
 28 H Isotropic = 30.3408 Anisotropy = 10.0018
 XX= 28.9758 YX= 3.8323 ZX= -3.5217
 XY= 2.6046 YY= 30.6151 ZY= -3.4861

XZ= -2.2060 YZ= -3.8636 ZZ= 31.4316
 Eigenvalues: 26.4742 27.5396 37.0087
 29 H Isotropic = 29.9337 Anisotropy = 9.6442
 XX= 27.6504 YX= -1.1983 ZX= -0.9764
 XY= -1.6072 YY= 34.6746 ZY= 3.1216
 XZ= -1.2777 YZ= 3.6669 ZZ= 27.4761
 Eigenvalues: 25.9313 27.5066 36.3632
 30 H Isotropic = 30.8608 Anisotropy = 9.3675
 XX= 32.6842 YX= -2.9562 ZX= 4.2804
 XY= -3.5104 YY= 30.6032 ZY= -1.1985
 XZ= 3.8815 YZ= -1.0149 ZZ= 29.2949
 Eigenvalues: 26.3223 29.1543 37.1058
 31 H Isotropic = 30.5179 Anisotropy = 10.1839
 XX= 29.6653 YX= -1.4837 ZX= -5.8298
 XY= -2.1345 YY= 29.7881 ZY= 1.3275
 XZ= -5.8148 YZ= 0.5919 ZZ= 32.1002
 Eigenvalues: 24.7986 29.4479 37.3071
 32 H Isotropic = 30.7164 Anisotropy = 8.6193
 XX= 30.8655 YX= 1.4716 ZX= -1.3344
 XY= 1.7803 YY= 35.8192 ZY= 1.9307
 XZ= -2.0720 YZ= 1.7368 ZZ= 25.4644
 Eigenvalues: 24.5319 31.1546 36.4626
 33 H Isotropic = 29.8520 Anisotropy = 10.7327
 XX= 32.0406 YX= -0.0880 ZX= 5.1471
 XY= -0.7411 YY= 25.5585 ZY= 0.4779
 XZ= 4.8469 YZ= 1.3752 ZZ= 31.9569
 Eigenvalues: 25.0786 27.4702 37.0072
 34 H Isotropic = 29.0064 Anisotropy = 8.7025
 XX= 29.5318 YX= 1.3966 ZX= 0.8983
 XY= 1.1169 YY= 34.0590 ZY= 2.3880
 XZ= -0.7523 YZ= 2.1016 ZZ= 23.4284
 Eigenvalues: 22.9689 29.2422 34.8081
 35 H Isotropic = 28.6357 Anisotropy = 11.0523
 XX= 35.5396 YX= 0.4475 ZX= -2.1775
 XY= 2.3994 YY= 26.0498 ZY= 0.7580
 XZ= -1.5341 YZ= 0.8528 ZZ= 24.3176
 Eigenvalues: 23.5733 26.3298 36.0038
 36 H Isotropic = 29.2250 Anisotropy = 6.7589
 XX= 27.4522 YX= 0.5143 ZX= -1.7705
 XY= 0.8503 YY= 29.9534 ZY= -3.8047
 XZ= -2.5549 YZ= -2.0690 ZZ= 30.2692
 Eigenvalues: 26.0116 27.9324 33.7309
 37 H Isotropic = 27.7726 Anisotropy = 10.8170
 XX= 26.6824 YX= -2.1205 ZX= -1.4376
 XY= -3.6230 YY= 28.9977 ZY= 5.4045
 XZ= -1.6171 YZ= 5.4173 ZZ= 27.6378
 Eigenvalues: 22.6806 25.6533 34.9839
 38 H Isotropic = 28.3323 Anisotropy = 7.0634
 XX= 26.2630 YX= -0.7228 ZX= -0.0142
 XY= 1.3679 YY= 25.7612 ZY= 0.0974
 XZ= -1.3468 YZ= -0.1089 ZZ= 32.9727
 Eigenvalues: 25.5910 26.3647 33.0412
 39 H Isotropic = 29.4173 Anisotropy = 5.4157
 XX= 30.7813 YX= -1.0393 ZX= -1.0645
 XY= -1.7808 YY= 31.6654 ZY= 0.7756
 XZ= -1.0196 YZ= 1.5033 ZZ= 25.8051
 Eigenvalues: 25.4727 29.7514 33.0277
 40 H Isotropic = 29.9794 Anisotropy = 5.7559
 XX= 28.8565 YX= 1.0971 ZX= 1.3498
 XY= 1.4313 YY= 29.1890 ZY= -2.5633
 XZ= 1.2531 YZ= -3.3206 ZZ= 31.8927
 Eigenvalues: 26.1433 29.9782 33.8167
 41 H Isotropic = 27.7304 Anisotropy = 7.1683
 XX= 27.1453 YX= -1.2955 ZX= -0.3054
 XY= -1.6560 YY= 27.4572 ZY= -5.4668
 XZ= -0.2934 YZ= -3.2156 ZZ= 28.5887
 Eigenvalues: 23.2051 27.4769 32.5093
 42 H Isotropic = 26.1051 Anisotropy = 6.2071
 XX= 25.9601 YX= -0.2714 ZX= -0.6041
 XY= 0.5054 YY= 30.2339 ZY= 1.3900
 XZ= -0.5450 YZ= -0.9169 ZZ= 22.1212
 Eigenvalues: 22.0294 26.0427 30.2432
 43 H Isotropic = 28.4195 Anisotropy = 6.4154
 XX= 28.9546 YX= 4.2944 ZX= 0.1274

XY= 3.9961 YY= 27.9287 ZY= -0.6625
 XZ= 0.4560 YZ= 1.7532 ZZ= 28.3750
 Eigenvalues: 24.2534 28.3085 32.6964
 44 H Isotropic = 27.9959 Anisotropy = 5.1638
 XX= 31.2708 YX= -1.3816 ZX= -0.8144
 XY= -0.5991 YY= 25.5641 ZY= -0.1004
 XZ= 0.4232 YZ= -1.5681 ZZ= 27.1528
 Eigenvalues: 25.0494 27.4999 31.4385
 45 H Isotropic = 26.9840 Anisotropy = 3.8092
 XX= 26.7496 YX= -0.6136 ZX= -0.0578
 XY= -0.8758 YY= 24.8566 ZY= -1.4373
 XZ= -0.5816 YZ= -0.3208 ZZ= 29.3457
 Eigenvalues: 24.4211 27.0074 29.5234
 46 H Isotropic = 29.6854 Anisotropy = 4.9401
 XX= 31.8669 YX= -0.0716 ZX= 1.9598
 XY= -0.5639 YY= 28.4304 ZY= -1.0236
 XZ= 1.5373 YZ= -3.0969 ZZ= 28.7588
 Eigenvalues: 26.3462 29.7311 32.9788
 47 H Isotropic = 25.0678 Anisotropy = 4.6752
 XX= 24.9794 YX= -2.0335 ZX= -2.8817
 XY= -1.1390 YY= 23.7949 ZY= 0.1424
 XZ= 0.5566 YZ= 3.0922 ZZ= 26.4292
 Eigenvalues: 22.5407 24.4782 28.1846
 48 H Isotropic = 25.6002 Anisotropy = 8.1491
 XX= 24.0963 YX= 3.0523 ZX= -0.6869
 XY= 2.8082 YY= 29.3532 ZY= -1.3249
 XZ= -0.4360 YZ= -1.8743 ZZ= 23.3510
 Eigenvalues: 22.7176 23.0501 31.0329
 49 H Isotropic = 28.8205 Anisotropy = 19.4943
 XX= 24.4779 YX= -5.5429 ZX= 0.2265
 XY= -5.6744 YY= 30.7341 ZY= 9.3912
 XZ= -0.7828 YZ= 10.2177 ZZ= 31.2495
 Eigenvalues: 18.4243 26.2205 41.8167
 50 H Isotropic = 30.5255 Anisotropy = 18.1373
 XX= 36.2486 YX= -10.4793 ZX= -0.5029
 XY= -9.4366 YY= 26.6856 ZY= -2.6358
 XZ= 0.8358 YZ= -1.3345 ZZ= 28.6425
 Eigenvalues: 20.1211 28.8385 42.6171

Structure Coordinates of Caulamidine A from DFT Geometry Optimization

C	4.021	-1.026	-1.527
C	2.729	-0.675	-1.109
C	2.528	-0.27	0.227
C	3.604	-0.21	1.11
C	4.88	-0.556	0.667
C	5.099	-0.967	-0.648
N	1.679	-0.761	-2.029
C	0.556	-0.161	-1.783
C	1.11	0.02	0.638
C	-1.199	0.796	-0.128
C	0.313	0.675	-0.515
C	-1.377	1.864	0.964
N	-0.817	3.101	0.798
C	0.567	3.135	0.291
C	0.849	2.113	-0.814
N	-2.105	1.506	1.978
C	-1.108	4.099	1.823
Cl	6.236	-0.471	1.789
C	-2.429	0.151	1.763
C	-1.864	-0.372	0.58
C	-2.005	-1.713	0.255
C	-2.747	-2.522	1.127
C	-3.33	-2.012	2.286
C	-3.17	-0.662	2.615
Cl	-2.94	-4.231	0.742
C	-1.967	1.212	-1.41
N	-0.409	-0.151	-2.764
C	-1.811	0.17	-2.509
C	-0.158	-0.89	-3.999
Cl	-3.745	1.483	-1.142

H	-1.604	2.181	-1.747
H	-2.173	4.074	2.055
H	-0.837	5.086	1.441
H	-0.552	3.908	2.752
H	0.895	-0.803	-4.259
H	-0.78	-0.469	-4.794
H	-0.394	-1.957	-3.892
H	0.617	-0.921	0.908
H	1.074	0.651	1.533
H	0.761	4.141	-0.094
H	1.261	2.982	1.133
H	0.436	2.469	-1.761
H	1.933	2.059	-0.955
H	-2.243	0.565	-3.433
H	-2.387	-0.728	-2.245
H	4.162	-1.342	-2.556
H	3.453	0.098	2.14
H	6.097	-1.234	-0.976
H	-1.55	-2.151	-0.627
H	-3.899	-2.671	2.933
H	-3.605	-0.254	3.52

GIAO Chemical Shielding Tensors of Caulamidine A

1 C Isotropic = 73.3703 Anisotropy = 141.2073
 XX= 61.7645 YX= 20.1256 ZX= 8.3978
 XY= 22.6134 YY= 150.8281 ZY= -45.4062
 XZ= 4.3523 YZ= -46.0083 ZZ= 7.5184
 Eigenvalues: -7.9826 60.5851 167.5086

2 C Isotropic = 56.1240 Anisotropy = 151.0068
 XX= 2.2535 YX= 21.9017 ZX= -31.7615
 XY= 5.5815 YY= 147.1450 ZY= -30.3660
 XZ= -38.4038 YZ= -29.5607 ZZ= 18.9735
 Eigenvalues: -25.8332 37.4100 156.7952

3 C Isotropic = 73.9681 Anisotropy = 155.5631
 XX= 11.4624 YX= 28.4309 ZX= 14.6050
 XY= 30.6791 YY= 164.5843 ZY= -31.0167
 XZ= 7.3042 YZ= -36.9867 ZZ= 45.8575
 Eigenvalues: -1.0643 45.2916 177.6768

4 C Isotropic = 72.1485 Anisotropy = 124.9639
 XX= 71.4064 YX= 14.7081 ZX= 6.0047
 XY= 8.8009 YY= 141.5472 ZY= -44.4196
 XZ= 12.3490 YZ= -44.2133 ZZ= 3.4921
 Eigenvalues: -11.2938 72.2816 155.4578

5 C Isotropic = 62.7872 Anisotropy = 96.2986
 XX= 23.5580 YX= 4.1230 ZX= -47.1358
 XY= 5.5475 YY= 122.6791 ZY= -11.9696
 XZ= -47.2617 YZ= -15.7686 ZZ= 42.1245
 Eigenvalues: -15.4510 76.8263 126.9863

6 C Isotropic = 71.0978 Anisotropy = 141.3478
 XX= 1.3397 YX= 33.9428 ZX= 19.4546
 XY= 34.0807 YY= 150.8592 ZY= -30.3426
 XZ= 16.5239 YZ= -32.1980 ZZ= 61.0945
 Eigenvalues: -14.2618 62.2255 165.3297

7 N Isotropic = 30.5974 Anisotropy = 329.5536
 XX= -90.3982 YX= 72.9496 ZX= -107.6496
 XY= 101.8368 YY= 176.1129 ZY= -78.8872
 XZ= -107.6878 YZ= -74.5075 ZZ= 6.0775
 Eigenvalues: -163.6262 5.1186 250.2998

8 C Isotropic = 42.1054 Anisotropy = 122.4684
 XX= 36.7657 YX= 10.4281 ZX= -55.4613
 XY= 38.1858 YY= 90.2246 ZY= -33.8850
 XZ= -19.9424 YZ= -52.5531 ZZ= -0.6742
 Eigenvalues: -29.8249 32.3900 123.7510

9 C Isotropic = 163.9295 Anisotropy = 30.7497
 XX= 183.1890 YX= -9.7276 ZX= -2.1628
 XY= -2.3796 YY= 149.9786 ZY= -7.5451
 XZ= 4.2144 YZ= -4.5715 ZZ= 158.6209
 Eigenvalues: 146.1904 161.1687 184.4293

10 C Isotropic = 133.6350 Anisotropy = 8.4992
 XX= 132.1560 YX= 0.4894 ZX= 2.3603
 XY= 2.4525 YY= 138.5751 ZY= -3.1071

XZ= -0.3945 YZ= -1.1990 ZZ= 130.1738
 Eigenvalues: 129.0778 132.5260 139.3011
 11 C Isotropic = 149.8353 Anisotropy = 10.5135
 XX= 150.8640 YX= 6.5660 ZX= -1.5064
 XY= 0.6875 YY= 154.3546 ZY= 5.0037
 XZ= -4.6389 YZ= 2.2930 ZZ= 144.2872
 Eigenvalues: 141.3115 151.3500 156.8443
 12 C Isotropic = 25.6525 Anisotropy = 119.8213
 XX= 61.0411 YX= -45.6530 ZX= 34.0583
 XY= -22.0725 YY= -24.2707 ZY= -58.7191
 XZ= 29.5146 YZ= -26.0970 ZZ= 40.1869
 Eigenvalues: -48.1664 19.5904 105.5333
 13 N Isotropic = 178.6561 Anisotropy = 57.0590
 XX= 179.2225 YX= 16.6399 ZX= 34.0686
 XY= -3.7729 YY= 206.5919 ZY= 8.9946
 XZ= 54.6386 YZ= -1.7402 ZZ= 150.1540
 Eigenvalues: 118.0060 201.2669 216.6954
 14 C Isotropic = 146.4623 Anisotropy = 52.3242
 XX= 172.5768 YX= 3.0525 ZX= -21.9418
 XY= 1.9261 YY= 131.6762 ZY= 9.6545
 XZ= -18.1439 YZ= 10.5424 ZZ= 135.1341
 Eigenvalues: 118.4499 139.5919 181.3452
 15 C Isotropic = 168.0703 Anisotropy = 18.5335
 XX= 154.2974 YX= 10.3105 ZX= -8.0709
 XY= -4.0269 YY= 177.7419 ZY= 2.0173
 XZ= 1.3805 YZ= 7.2840 ZZ= 172.1715
 Eigenvalues: 153.0483 170.7366 180.4259
 16 N Isotropic = 1.8926 Anisotropy = 324.9541
 XX= 109.3593 YX= -142.5246 ZX= 88.8207
 XY= -130.9505 YY= -145.5634 ZY= -10.5896
 XZ= 118.5731 YZ= 24.8457 ZZ= 41.8819
 Eigenvalues: -214.8154 1.9646 218.5287
 17 C Isotropic = 157.1465 Anisotropy = 53.7879
 XX= 142.9931 YX= -8.8105 ZX= -6.3505
 XY= -14.4810 YY= 166.4434 ZY= 25.7413
 XZ= -9.1196 YZ= 23.9804 ZZ= 162.0031
 Eigenvalues: 137.1422 141.2923 193.0051
 18 Cl Isotropic = 745.6722 Anisotropy = 445.7861
 XX= 857.7816 YX= 20.1521 ZX= 222.5571
 XY= 17.9074 YY= 606.9492 ZY= 11.0637
 XZ= 222.9181 YZ= 9.2948 ZZ= 772.2857
 Eigenvalues: 587.2543 606.8993 1042.8629
 19 C Isotropic = 42.6006 Anisotropy = 133.3178
 XX= 104.8531 YX= -19.7264 ZX= 32.8428
 XY= -32.9676 YY= -27.9125 ZY= -24.0419
 XZ= 38.3681 YZ= -38.1621 ZZ= 50.8613
 Eigenvalues: -40.0820 36.4047 131.4792
 20 C Isotropic = 64.8497 Anisotropy = 140.7011
 XX= 109.2979 YX= -33.8811 ZX= 70.7649
 XY= -33.1744 YY= 27.3681 ZY= 4.6508
 XZ= 60.6524 YZ= 8.7023 ZZ= 57.8830
 Eigenvalues: -6.5843 42.4829 158.6504
 21 C Isotropic = 74.9504 Anisotropy = 134.3850
 XX= 124.2024 YX= 0.8888 ZX= 63.4456
 XY= -5.8062 YY= 55.9753 ZY= -31.4389
 XZ= 68.0744 YZ= -34.6500 ZZ= 44.6735
 Eigenvalues: -5.2541 65.5649 164.5404
 22 C Isotropic = 63.0850 Anisotropy = 95.0787
 XX= 110.5856 YX= -21.6542 ZX= 17.3036
 XY= -19.1233 YY= -7.8558 ZY= -23.7352
 XZ= 18.1375 YZ= -24.2073 ZZ= 86.5251
 Eigenvalues: -15.6206 78.4047 126.4708
 23 C Isotropic = 69.0081 Anisotropy = 145.8769
 XX= 111.3271 YX= -44.5049 ZX= 70.7496
 XY= -41.9390 YY= 36.3844 ZY= 12.9909
 XZ= 69.3082 YZ= 14.8894 ZZ= 59.3127
 Eigenvalues: -16.3294 57.0944 166.2593
 24 C Isotropic = 78.7263 Anisotropy = 147.2814
 XX= 131.5354 YX= -12.2772 ZX= 69.1256
 XY= -12.2632 YY= 56.5800 ZY= -33.2231
 XZ= 70.0949 YZ= -30.7667 ZZ= 48.0635
 Eigenvalues: -0.3500 59.6151 176.9139
 25 Cl Isotropic = 744.3695 Anisotropy = 449.2518
 XX= 606.3369 YX= 44.4931 ZX= 7.9014

XY= 46.1914 YY= 1017.6208 ZY= 97.2326
 XZ= 16.9450 YZ= 93.6977 ZZ= 609.1508
 Eigenvalues: 587.5620 601.6758 1043.8707
 26 C Isotropic = 131.9597 Anisotropy = 37.9082
 XX= 155.8470 YX= -3.7316 ZX= 0.6133
 XY= 0.2230 YY= 103.6539 ZY= 1.3887
 XZ= -10.9790 YZ= 2.7745 ZZ= 136.3782
 Eigenvalues: 103.4827 135.1646 157.2318
 27 N Isotropic = 168.4667 Anisotropy = 63.9112
 XX= 146.8593 YX= 31.1782 ZX= 41.2037
 XY= 27.8584 YY= 165.3508 ZY= -15.8643
 XZ= 24.7464 YZ= -3.3920 ZZ= 193.1901
 Eigenvalues: 112.0381 182.2880 211.0742
 28 C Isotropic = 142.1216 Anisotropy = 55.2026
 XX= 165.5857 YX= -16.7552 ZX= -11.1831
 XY= -17.0915 YY= 126.2872 ZY= 10.2945
 XZ= -17.2476 YZ= 14.0455 ZZ= 134.4918
 Eigenvalues: 116.6099 130.8314 178.9233
 29 C Isotropic = 158.5209 Anisotropy = 51.2351
 XX= 139.0610 YX= -3.0297 ZX= -7.1055
 XY= -10.0630 YY= 153.8083 ZY= 16.0405
 XZ= -10.2752 YZ= 17.9747 ZZ= 182.6934
 Eigenvalues: 136.4199 146.4652 192.6777
 30 Cl Isotropic = 825.2891 Anisotropy = 398.7389
 XX= 1067.8549 YX= -88.1460 ZX= -36.1264
 XY= -66.6517 YY= 691.7209 ZY= 24.1388
 XZ= -61.5745 YZ= 43.7720 ZZ= 716.2915
 Eigenvalues: 663.8824 720.8699 1091.1150
 31 H Isotropic = 26.9536 Anisotropy = 5.4980
 XX= 29.8788 YX= 1.5543 ZX= 0.9342
 XY= 1.6556 YY= 26.9053 ZY= -1.4178
 XZ= -0.3150 YZ= -2.3721 ZZ= 24.0767
 Eigenvalues: 22.9752 27.2667 30.6189
 32 H Isotropic = 28.0650 Anisotropy = 10.4456
 XX= 30.1133 YX= -2.0861 ZX= -3.6483
 XY= -3.1952 YY= 28.3072 ZY= 4.2407
 XZ= -4.1561 YZ= 2.9942 ZZ= 25.7745
 Eigenvalues: 22.6684 26.4978 35.0287
 33 H Isotropic = 29.5112 Anisotropy = 10.8451
 XX= 25.0117 YX= -0.6675 ZX= -1.1310
 XY= -0.0672 YY= 36.4224 ZY= 1.0397
 XZ= -0.8780 YZ= 2.3251 ZZ= 27.0994
 Eigenvalues: 24.5992 27.1930 36.7413
 34 H Isotropic = 29.0133 Anisotropy = 10.5733
 XX= 25.3539 YX= 0.2474 ZX= 1.7516
 XY= -0.1575 YY= 27.5358 ZY= 4.0078
 XZ= 2.4191 YZ= 3.1407 ZZ= 34.1504
 Eigenvalues: 24.5705 26.4073 36.0622
 35 H Isotropic = 27.2668 Anisotropy = 9.9417
 XX= 30.0622 YX= -0.6155 ZX= -2.5279
 XY= -1.5669 YY= 21.4167 ZY= 2.0695
 XZ= -3.9125 YZ= 2.5936 ZZ= 30.3215
 Eigenvalues: 20.8327 27.0731 33.8946
 36 H Isotropic = 29.6406 Anisotropy = 10.3484
 XX= 26.1726 YX= -1.4245 ZX= 0.7071
 XY= -1.5115 YY= 26.4451 ZY= 0.7749
 XZ= 2.3895 YZ= 0.0732 ZZ= 36.3041
 Eigenvalues: 24.6564 27.7259 36.5395
 37 H Isotropic = 28.8680 Anisotropy = 10.8856
 XX= 24.2393 YX= 0.6753 ZX= -0.6464
 XY= 1.2875 YY= 33.8310 ZY= 3.7728
 XZ= -0.7149 YZ= 4.5161 ZZ= 28.5335
 Eigenvalues: 23.7602 26.7186 36.1250
 38 H Isotropic = 29.0276 Anisotropy = 10.6224
 XX= 35.3426 YX= 1.4134 ZX= -2.1505
 XY= 2.6187 YY= 28.0268 ZY= -4.2969
 XZ= 0.6384 YZ= -3.1095 ZZ= 23.7134
 Eigenvalues: 21.5754 29.3982 36.1092
 39 H Isotropic = 29.7828 Anisotropy = 5.9403
 XX= 31.8159 YX= -1.7767 ZX= 0.6611
 XY= -3.0972 YY= 26.0882 ZY= 2.2371
 XZ= 3.5257 YZ= 2.3867 ZZ= 31.4443
 Eigenvalues: 24.0377 31.5678 33.7430
 40 H Isotropic = 28.8647 Anisotropy = 9.0542

XX= 27.0462 YX= 4.0491 ZX= -2.9172
 XY= 1.2815 YY= 33.8819 ZY= 0.1657
 XZ= -2.2185 YZ= -0.3843 ZZ= 25.6660
 Eigenvalues: 23.4511 28.2422 34.9009
 41 H Isotropic = 28.7092 Anisotropy = 7.4608
 XX= 32.0266 YX= 0.6688 ZX= 3.3941
 XY= -1.2609 YY= 27.2452 ZY= 4.0218
 XZ= 2.6607 YZ= 2.8103 ZZ= 26.8558
 Eigenvalues: 22.9575 29.4871 33.6831
 42 H Isotropic = 29.7416 Anisotropy = 6.1177
 XX= 26.1179 YX= 2.4225 ZX= 0.0154
 XY= -0.1327 YY= 30.5919 ZY= -2.0349
 XZ= 2.1269 YZ= -2.0438 ZZ= 32.5151
 Eigenvalues: 25.4854 29.9195 33.8201
 43 H Isotropic = 29.9960 Anisotropy = 7.2667
 XX= 33.9750 YX= 0.3413 ZX= -2.7971
 XY= -2.6364 YY= 31.1269 ZY= 0.3502
 XZ= -1.8709 YZ= -0.8745 ZZ= 24.8860
 Eigenvalues: 24.2809 30.8665 34.8404
 44 H Isotropic = 28.5233 Anisotropy = 7.6006
 XX= 28.3106 YX= -3.4353 ZX= 3.0521
 XY= -2.8245 YY= 24.3881 ZY= -0.0126
 XZ= 0.6269 YZ= 0.6758 ZZ= 32.8711
 Eigenvalues: 22.5173 29.4622 33.5904
 45 H Isotropic = 28.0484 Anisotropy = 4.0128
 XX= 28.0204 YX= 2.9271 ZX= 0.4015
 XY= 2.3852 YY= 28.1132 ZY= 0.7291
 XZ= -2.2452 YZ= 1.0154 ZZ= 28.0116
 Eigenvalues: 24.8938 28.5278 30.7236
 46 H Isotropic = 24.5374 Anisotropy = 6.5512
 XX= 28.5921 YX= -1.7171 ZX= 0.3344
 XY= -1.3646 YY= 21.0710 ZY= 1.2504
 XZ= 0.6082 YZ= 1.3616 ZZ= 23.9492
 Eigenvalues: 20.2567 24.4507 28.9049
 47 H Isotropic = 24.9006 Anisotropy = 11.2089
 XX= 31.6052 YX= -1.8748 ZX= 1.7725
 XY= -2.0262 YY= 20.1046 ZY= 0.6602
 XZ= 2.5401 YZ= 0.4247 ZZ= 22.9922
 Eigenvalues: 19.5315 22.7972 32.3733
 48 H Isotropic = 24.4840 Anisotropy = 5.9518
 XX= 25.0908 YX= -0.6856 ZX= 1.2924
 XY= -0.8746 YY= 20.7083 ZY= 2.1289
 XZ= 0.7234 YZ= 2.2150 ZZ= 27.6530
 Eigenvalues: 19.8796 25.1206 28.4519
 49 H Isotropic = 24.7006 Anisotropy = 12.1858
 XX= 21.6119 YX= 3.1805 ZX= -2.7905
 XY= 5.1495 YY= 29.8404 ZY= -2.7189
 XZ= -2.8492 YZ= -2.5623 ZZ= 22.6494
 Eigenvalues: 18.9487 22.3286 32.8245
 50 H Isotropic = 24.3207 Anisotropy = 6.0724
 XX= 21.5565 YX= 0.4059 ZX= -2.9132
 XY= 0.4218 YY= 25.8285 ZY= 2.2790
 XZ= -3.0551 YZ= 1.9485 ZZ= 25.5772
 Eigenvalues: 19.6509 24.9423 28.3690
 51 H Isotropic = 24.2814 Anisotropy = 4.8745
 XX= 22.2474 YX= 1.7701 ZX= -2.7518
 XY= 1.9463 YY= 25.9261 ZY= -0.3684
 XZ= -2.6241 YZ= -0.1247 ZZ= 24.6706
 Eigenvalues: 20.1435 25.1695 27.5310

Structure Coordinates of the C26-inverted diastereomer of Caulamidine A from DFT Geometry Optimization

C	3.938	0.683	1.67
C	2.64	0.457	1.188
C	2.426	0.406	-0.205
C	3.495	0.567	-1.084
C	4.777	0.782	-0.578
C	5.009	0.843	0.796
Cl	6.124	0.978	-1.698
N	1.598	0.317	2.112
C	0.465	-0.187	1.732

C	1.003	0.233	-0.665
N	-0.495	-0.439	2.687
C	-1.915	-0.522	2.362
C	-2.21	-1.245	1.054
C	-1.292	-0.705	-0.095
C	0.21	-0.683	0.299
C	-0.206	-0.068	4.069
Cl	-2.192	-3.062	1.342
C	-1.52	-1.498	-1.396
N	-0.89	-2.678	-1.606
C	0.467	-2.875	-1.075
C	0.753	-2.145	0.24
C	-1.19	-3.404	-2.834
N	-2.353	-0.949	-2.239
C	-2.648	0.321	-1.721
C	-1.967	0.603	-0.515
C	-2.058	1.853	0.081
C	-2.86	2.819	-0.541
C	-3.559	2.546	-1.716
C	-3.455	1.288	-2.318
Cl	-2.981	4.419	0.187
H	-0.367	1.004	4.25
H	0.837	-0.29	4.288
H	-0.86	-0.642	4.73
H	-0.64	-2.996	-3.693
H	-2.256	-3.329	-3.045
H	-0.912	-4.453	-2.7
H	0.517	1.216	-0.696
H	0.961	-0.16	-1.686
H	-2.42	-1.044	3.177
H	-2.363	0.481	2.302
H	0.616	-3.949	-0.923
H	1.188	-2.564	-1.848
H	0.34	-2.712	1.073
H	1.839	-2.12	0.375
H	-3.247	-1.06	0.774
H	4.089	0.726	2.744
H	3.335	0.531	-2.157
H	6.012	1.012	1.171
H	-1.517	2.108	0.986
H	-4.174	3.319	-2.165
H	-3.978	1.068	-3.242

GIAO Chemical Shielding Tensors of the C26-inverted diastereomer of Caulamidine A

1 C Isotropic = 73.0726 Anisotropy = 141.7364

XX= 60.9556 YX= -16.8315 ZX= -14.1683

XY= -20.4953 YY= 164.2705 ZY= -3.9181

XZ= -10.5147 YZ= -4.6094 ZZ= -6.0084

Eigenvalues: -8.5422 60.1964 167.5635

2 C Isotropic = 55.9566 Anisotropy = 150.8524

XX= 2.5270 YX= -27.9479 ZX= 25.4012

XY= -14.4584 YY= 153.5974 ZY= 4.8041

XZ= 35.5276 YZ= 5.7110 ZZ= 11.7454

Eigenvalues: -25.8132 37.1582 156.5249

3 C Isotropic = 73.5236 Anisotropy = 155.4043

XX= 10.5344 YX= -22.8742 ZX= -21.5142

XY= -27.0330 YY= 173.3245 ZY= 3.8577

XZ= -14.5661 YZ= -3.2979 ZZ= 36.7119

Eigenvalues: -1.5053 44.9497 177.1265

4 C Isotropic = 71.9046 Anisotropy = 124.9891

XX= 71.0436 YX= -12.2261 ZX= -10.2891

XY= -5.1612 YY= 154.2610 ZY= -5.0282

XZ= -15.2088 YZ= -4.4484 ZZ= -9.5907

Eigenvalues: -11.7769 72.2600 155.2307

5 C Isotropic = 62.4500 Anisotropy = 96.5695

XX= 23.6753 YX= -15.3945 ZX= 44.9970

XY= -16.1215 YY= 124.4183 ZY= 8.9655

XZ= 44.6038 YZ= 5.7917 ZZ= 39.2565

Eigenvalues: -16.0218 76.5421 126.8297

6 C Isotropic = 71.2329 Anisotropy = 141.2294

XX= 0.6765 YX= -26.9316 ZX= -27.0433

XY= -27.8733 YY= 160.8251 ZY= -3.7914
 XZ= -24.2809 YZ= -5.6329 ZZ= 52.1970
 Eigenvalues: -14.1415 62.4543 165.3858
 7 Cl Isotropic = 745.2450 Anisotropy = 446.2478
 XX= 853.8384 YX= 35.6811 ZX= -221.4033
 XY= 37.7094 YY= 611.8026 ZY= -30.2275
 XZ= -221.5818 YZ= -31.8769 ZZ= 770.0941
 Eigenvalues: 586.5384 606.4532 1042.7435
 8 N Isotropic = 26.1567 Anisotropy = 335.8053
 XX= -98.8232 YX= -95.4050 ZX= 87.3591
 XY= -126.4314 YY= 204.6895 ZY= -24.8479
 XZ= 78.1603 YZ= -24.4276 ZZ= -27.3963
 Eigenvalues: -171.5198 -0.0371 250.0268
 9 C Isotropic = 40.6238 Anisotropy = 125.4938
 XX= 33.3926 YX= -23.6023 ZX= 50.1005
 XY= -43.0142 YY= 107.1832 ZY= -3.9342
 XZ= 9.7521 YZ= -25.2015 ZZ= -18.7045
 Eigenvalues: -32.3334 29.9184 124.2863
 10 C Isotropic = 162.8777 Anisotropy = 30.0302
 XX= 181.8235 YX= 8.7794 ZX= 4.2004
 XY= 2.1444 YY= 153.8293 ZY= -8.7429
 XZ= -3.5261 YZ= -7.1401 ZZ= 152.9804
 Eigenvalues: 145.0066 160.7287 182.8979
 11 N Isotropic = 175.9394 Anisotropy = 67.1626
 XX= 147.0520 YX= -18.5302 ZX= -53.5811
 XY= -28.2229 YY= 186.6066 ZY= -14.8983
 XZ= -34.5243 YZ= -8.3281 ZZ= 194.1595
 Eigenvalues: 111.6175 195.4862 220.7144
 12 C Isotropic = 140.2180 Anisotropy = 28.4338
 XX= 150.0455 YX= 13.1354 ZX= 9.8243
 XY= 4.6848 YY= 129.4941 ZY= 3.4935
 XZ= 7.2466 YZ= 8.9280 ZZ= 141.1145
 Eigenvalues: 125.4945 135.9857 159.1739
 13 C Isotropic = 128.8183 Anisotropy = 49.9079
 XX= 95.8642 YX= -1.8113 ZX= -16.3194
 XY= -15.9384 YY= 157.9407 ZY= -6.3444
 XZ= -8.7745 YZ= -14.9197 ZZ= 132.6501
 Eigenvalues: 89.9710 134.3938 162.0903
 14 C Isotropic = 133.7180 Anisotropy = 18.6175
 XX= 123.7419 YX= 2.5494 ZX= -4.2646
 XY= -3.6369 YY= 145.9213 ZY= -2.9610
 XZ= 8.2795 YZ= -0.3013 ZZ= 131.4907
 Eigenvalues: 123.2518 131.7724 146.1296
 15 C Isotropic = 154.1476 Anisotropy = 12.1008
 XX= 150.1310 YX= -7.6120 ZX= -1.6769
 XY= -0.1831 YY= 160.1872 ZY= 4.0248
 XZ= 3.0396 YZ= 1.9806 ZZ= 152.1246
 Eigenvalues: 148.0615 152.1664 162.2148
 16 C Isotropic = 157.7108 Anisotropy = 50.8514
 XX= 140.0679 YX= 1.4964 ZX= 8.0717
 XY= 6.6306 YY= 145.0484 ZY= 6.0360
 XZ= 14.1620 YZ= 7.0967 ZZ= 188.0161
 Eigenvalues: 136.7266 144.7941 191.6117
 17 Cl Isotropic = 766.7292 Anisotropy = 412.8943
 XX= 598.9980 YX= 42.4141 ZX= -5.9603
 XY= 77.1979 YY= 1014.7092 ZY= -59.8360
 XZ= -65.5253 YZ= -95.1166 ZZ= 686.4805
 Eigenvalues: 583.6721 674.5235 1041.9921
 18 C Isotropic = 25.4558 Anisotropy = 122.5169
 XX= 47.4305 YX= 54.3451 ZX= -24.0093
 XY= 29.2342 YY= 9.8549 ZY= -71.3698
 XZ= -18.8449 YZ= -46.5102 ZZ= 19.0820
 Eigenvalues: -47.9317 17.1654 107.1338
 19 N Isotropic = 167.5346 Anisotropy = 63.2250
 XX= 155.6050 YX= -4.6320 ZX= -54.2999
 XY= 15.2596 YY= 192.8483 ZY= 13.2262
 XZ= -54.1783 YZ= 6.0392 ZZ= 154.1506
 Eigenvalues: 99.4325 193.4867 209.6847
 20 C Isotropic = 147.0466 Anisotropy = 50.3478
 XX= 171.7934 YX= -8.0007 ZX= 20.4559
 XY= -6.0492 YY= 128.8272 ZY= 7.6769
 XZ= 16.6398 YZ= 7.7454 ZZ= 140.5192
 Eigenvalues: 120.1968 140.3312 180.6118
 21 C Isotropic = 168.9768 Anisotropy = 14.1585

XX= 156.8056 YX= -11.6043 ZX= 6.7550
 XY= 3.1556 YY= 175.5379 ZY= 0.3226
 XZ= 0.6458 YZ= 6.2455 ZZ= 174.5869
 Eigenvalues: 154.9390 173.5756 178.4158
 22 C Isotropic = 157.7931 Anisotropy = 53.8240
 XX= 142.5332 YX= 7.0439 ZX= 8.2034
 XY= 11.8922 YY= 155.7796 ZY= 22.9205
 XZ= 12.8729 YZ= 21.9268 ZZ= 175.0664
 Eigenvalues: 137.5097 142.1937 193.6758
 23 N Isotropic = 19.2767 Anisotropy = 296.9113
 XX= 106.4120 YX= 141.4694 ZX= -44.3249
 XY= 147.8775 YY= -99.9986 ZY= -52.7645
 XZ= -85.9960 YZ= -32.8864 ZZ= 51.4169
 Eigenvalues: -174.8301 15.4427 217.2176
 24 C Isotropic = 43.6027 Anisotropy = 131.9071
 XX= 98.9899 YX= 21.9372 ZX= -33.8395
 XY= 37.8348 YY= -6.8267 ZY= -36.4741
 XZ= -39.6887 YZ= -46.9968 ZZ= 38.6448
 Eigenvalues: -32.0606 31.3278 131.5407
 25 C Isotropic = 61.6332 Anisotropy = 137.3777
 XX= 91.2892 YX= 39.9991 ZX= -73.7072
 XY= 36.7759 YY= 23.3759 ZY= -13.1472
 XZ= -50.6631 YZ= -3.1069 ZZ= 70.2345
 Eigenvalues: -2.1677 33.8490 153.2184
 26 C Isotropic = 75.1787 Anisotropy = 133.1197
 XX= 111.2542 YX= 11.6139 ZX= -68.5236
 XY= 15.9729 YY= 67.8689 ZY= -28.0302
 XZ= -71.2402 YZ= -31.1226 ZZ= 46.4129
 Eigenvalues: -2.8504 64.4613 163.9252
 27 C Isotropic = 65.0497 Anisotropy = 92.6541
 XX= 109.0294 YX= 21.1990 ZX= -14.5893
 XY= 17.6468 YY= 8.6163 ZY= -40.4671
 XZ= -16.5828 YZ= -43.1243 ZZ= 77.5034
 Eigenvalues: -12.1220 80.4519 126.8191
 28 C Isotropic = 68.8994 Anisotropy = 145.7432
 XX= 99.4149 YX= 56.8785 ZX= -64.5235
 XY= 55.3271 YY= 31.7291 ZY= 2.4198
 XZ= -63.2576 YZ= 4.1782 ZZ= 75.5542
 Eigenvalues: -16.2686 56.9053 166.0615
 29 C Isotropic = 79.0484 Anisotropy = 145.7763
 XX= 119.3513 YX= 24.1829 ZX= -69.6280
 XY= 22.9727 YY= 68.9400 ZY= -31.2888
 XZ= -73.8502 YZ= -29.2136 ZZ= 48.8540
 Eigenvalues: 1.2488 59.6639 176.2326
 30 Cl Isotropic = 746.2618 Anisotropy = 449.2430
 XX= 608.4787 YX= -26.8547 ZX= -5.6684
 XY= -23.9231 YY= 966.0381 ZY= 174.6832
 XZ= -20.8280 YZ= 169.1370 ZZ= 664.2687
 Eigenvalues: 586.2946 606.7337 1045.7572
 31 H Isotropic = 28.9001 Anisotropy = 11.0896
 XX= 24.2237 YX= -0.2555 ZX= 0.3893
 XY= -0.6789 YY= 31.5101 ZY= 4.7668
 XZ= 0.6749 YZ= 5.3281 ZZ= 30.9665
 Eigenvalues: 23.9949 26.4123 36.2932
 32 H Isotropic = 27.3619 Anisotropy = 9.9109
 XX= 29.9651 YX= -0.4537 ZX= 2.6419
 XY= 0.1138 YY= 21.2501 ZY= -0.7230
 XZ= 4.3674 YZ= -0.2396 ZZ= 30.8704
 Eigenvalues: 21.2261 26.8904 33.9692
 33 H Isotropic = 29.6070 Anisotropy = 10.3938
 XX= 26.1952 YX= 1.8074 ZX= -0.7443
 XY= 2.2310 YY= 26.7004 ZY= -1.3914
 XZ= -1.9545 YZ= -2.1331 ZZ= 35.9255
 Eigenvalues: 24.4106 27.8743 36.5362
 34 H Isotropic = 29.0500 Anisotropy = 10.7675
 XX= 25.4172 YX= 0.3726 ZX= -1.7401
 XY= 0.9949 YY= 26.0561 ZY= 1.7197
 XZ= -2.2989 YZ= 1.1940 ZZ= 35.6767
 Eigenvalues: 24.4319 26.4898 36.2284
 35 H Isotropic = 27.8186 Anisotropy = 10.4796
 XX= 29.8547 YX= 0.7275 ZX= 4.1666
 XY= 2.0011 YY= 26.1105 ZY= 4.1969
 XZ= 5.1044 YZ= 3.1951 ZZ= 27.4907
 Eigenvalues: 22.3285 26.3223 34.8050

36 H Isotropic = 29.4073 Anisotropy = 10.6345
 XX= 24.8652 YX= 0.4888 ZX= 1.3427
 XY= -0.1989 YY= 34.6916 ZY= 3.0466
 XZ= 0.8446 YZ= 4.3933 ZZ= 28.6650
 Eigenvalues: 24.4803 27.2446 36.4969
 37 H Isotropic = 29.0263 Anisotropy = 10.0074
 XX= 34.6552 YX= -1.9856 ZX= 1.6370
 XY= -2.6608 YY= 30.0600 ZY= -2.9541
 XZ= -1.5409 YZ= -1.7945 ZZ= 22.3637
 Eigenvalues: 21.6624 29.7186 35.6979
 38 H Isotropic = 29.8642 Anisotropy = 5.9386
 XX= 31.5221 YX= 1.9642 ZX= -0.1533
 XY= 3.9720 YY= 25.6185 ZY= 0.5313
 XZ= -2.8476 YZ= 0.7169 ZZ= 32.4520
 Eigenvalues: 24.2199 31.5495 33.8232
 39 H Isotropic = 28.4720 Anisotropy = 7.5985
 XX= 28.3086 YX= 3.2901 ZX= -4.1830
 XY= 2.1209 YY= 25.5675 ZY= 0.5455
 XZ= -1.9337 YZ= 0.2750 ZZ= 31.5398
 Eigenvalues: 23.3832 28.4950 33.5377
 40 H Isotropic = 27.6224 Anisotropy = 6.8133
 XX= 25.9434 YX= -3.8591 ZX= -1.7468
 XY= -4.9846 YY= 28.9917 ZY= 0.0283
 XZ= 1.2949 YZ= 0.3636 ZZ= 27.9323
 Eigenvalues: 22.7894 27.9133 32.1647
 41 H Isotropic = 28.7127 Anisotropy = 8.7067
 XX= 26.7708 YX= -4.2686 ZX= 1.3686
 XY= -1.6291 YY= 33.2221 ZY= 2.1163
 XZ= 1.4970 YZ= 1.3396 ZZ= 26.1452
 Eigenvalues: 23.8574 27.7636 34.5172
 42 H Isotropic = 28.6337 Anisotropy = 7.7090
 XX= 32.1196 YX= 0.0499 ZX= -3.4035
 XY= 1.8174 YY= 25.2512 ZY= 3.7017
 XZ= -2.3200 YZ= 2.5739 ZZ= 28.5303
 Eigenvalues: 22.7627 29.3654 33.7731
 43 H Isotropic = 28.7987 Anisotropy = 6.3427
 XX= 27.5215 YX= -0.5579 ZX= -1.3805
 XY= 2.3700 YY= 29.5225 ZY= -2.7021
 XZ= -3.2270 YZ= -2.5719 ZZ= 29.3521
 Eigenvalues: 25.7343 27.6347 33.0272
 44 H Isotropic = 30.0998 Anisotropy = 7.6128
 XX= 34.3046 YX= -0.5201 ZX= 2.3734
 XY= 2.3838 YY= 30.8911 ZY= 1.9042
 XZ= 2.1477 YZ= 0.6851 ZZ= 25.1036
 Eigenvalues: 24.4045 30.7198 35.1750
 45 H Isotropic = 27.9646 Anisotropy = 6.3038
 XX= 29.5260 YX= 0.9456 ZX= -1.4573
 XY= -3.2224 YY= 29.7933 ZY= -4.2581
 XZ= 1.4553 YZ= -3.3055 ZZ= 24.5746
 Eigenvalues: 22.5484 29.1783 32.1672
 46 H Isotropic = 24.4928 Anisotropy = 6.5158
 XX= 28.5241 YX= 1.7164 ZX= 0.0133
 XY= 1.4864 YY= 20.6077 ZY= 0.3579
 XZ= -0.3000 YZ= 0.4524 ZZ= 24.3466
 Eigenvalues: 20.2519 24.3898 28.8367
 47 H Isotropic = 24.8762 Anisotropy = 11.1019
 XX= 31.4931 YX= 2.2233 ZX= -1.2732
 XY= 2.5321 YY= 20.0388 ZY= -0.1269
 XZ= -2.0670 YZ= -0.3873 ZZ= 23.0968
 Eigenvalues: 19.5631 22.7880 32.2775
 48 H Isotropic = 24.4658 Anisotropy = 5.9668
 XX= 25.0480 YX= 0.9693 ZX= -1.0386
 XY= 0.9883 YY= 20.0704 ZY= 0.1332
 XZ= -0.4561 YZ= 0.2131 ZZ= 28.2789
 Eigenvalues: 19.8733 25.0804 28.4436
 49 H Isotropic = 24.8185 Anisotropy = 12.6255
 XX= 22.1256 YX= -4.5441 ZX= 1.7907
 XY= -5.8327 YY= 30.5622 ZY= -0.9342
 XZ= 1.5236 YZ= -0.8695 ZZ= 21.7677
 Eigenvalues: 19.1542 22.0658 33.2355
 50 H Isotropic = 24.3909 Anisotropy = 6.0922
 XX= 22.2968 YX= -0.7976 ZX= 3.1676
 XY= -0.7974 YY= 24.9888 ZY= 2.3042
 XZ= 3.2676 YZ= 1.9753 ZZ= 25.8871

Eigenvalues: 19.7744 24.9460 28.4524
 51 H Isotropic = 24.3909 Anisotropy = 4.8787
 XX= 22.9875 YX= -2.1806 ZX= 2.6375
 XY= -2.5389 YY= 26.0972 ZY= 0.2203
 XZ= 2.2698 YZ= 0.4870 ZZ= 24.0878
 Eigenvalues: 20.2613 25.2680 27.6433

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