Supporting information of

RCSA-Based Relative Stereochemical Analysis for Polar Molecules in PBLG Liquid Crystalline Medium

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PBLG Solubility and Alignment

The solubility of PBLG was measured in deuterium solvents by adding 3.75 mg PBLG to 600 µL acetone-d_6, 7.70 mg PBLG to 600 µL CD_3CN, 24.21 mg PBLG to 600 µL DMF-d_7, and 23.39 mg PBLG to 600 µL DMSO-d_6, respectively. After adding PBLG, the samples were mixed by inverting them more than 20 times. Each inversion was followed by a 2 min centrifugation to ensure that any undissolved PBLG settled at the bottom of the NMR tube. After mixing, PBLG retained its original appearance in acetone- d_6 and CD_3CN, while it became slightly viscous in DMF-d_7 and DMSO-d_6 (Figure S1). No significant change in fluidity was noted in acetone- d_6 and CD_3CN after the addition of PBLG; however, fluidity decreased in DMF-d_7 and DMSO-d_6. These results suggest that PBLG is insoluble in acetone-d_6 and CD_3CN, while its solubility in DMF-d_7 and DMSO- d_6 is limited, insufficient for achieving alignment, as indicated by the absence of RQC ^{2}H peaks in Figure S2.

Figure S1. NMR samples containing deuterium solvents and PBLG after mixing, from left to right a) Acetone-d_6 with 0.6% (w/v) PBLG, b) CD_3CN with 1.3% (w/v) PBLG, c) DMD-d_7 with 4.0% (w/v) PBLG, and d) DMSO-d_6 with 3.9% (w/v) PBLG.

Table S1. PBLG solubility and alignment in different deuterium solvents

Solvent	% (w/v) PBLG	Alignment
Acetone-d_6	N.D.	No
CD_3CN	N.D.	No
DMF-d_7	< 5.7	No
DMSO-d_6	< 4.5	No
THF-d_8	> 42.1	Yes

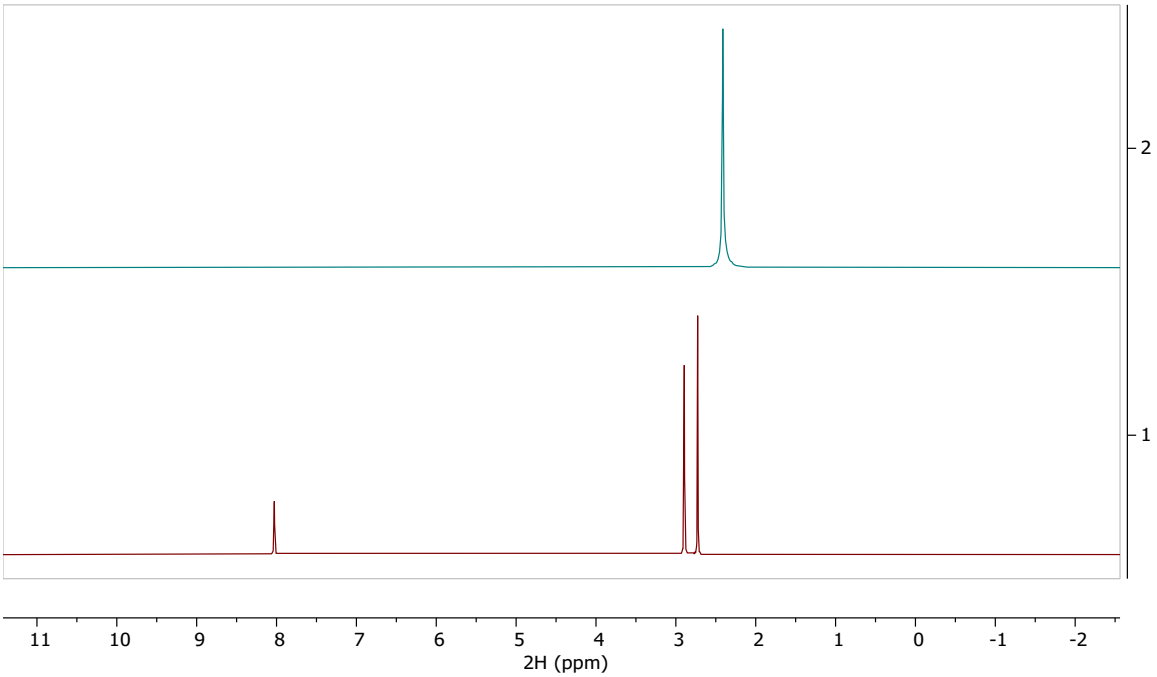


Figure S2. ^{2}H spectra of DMF-d_7 with 4.0% (w/v) PBLG (bottom) and DMSO-d_6 with 3.9% (w/v) PBLG (top).

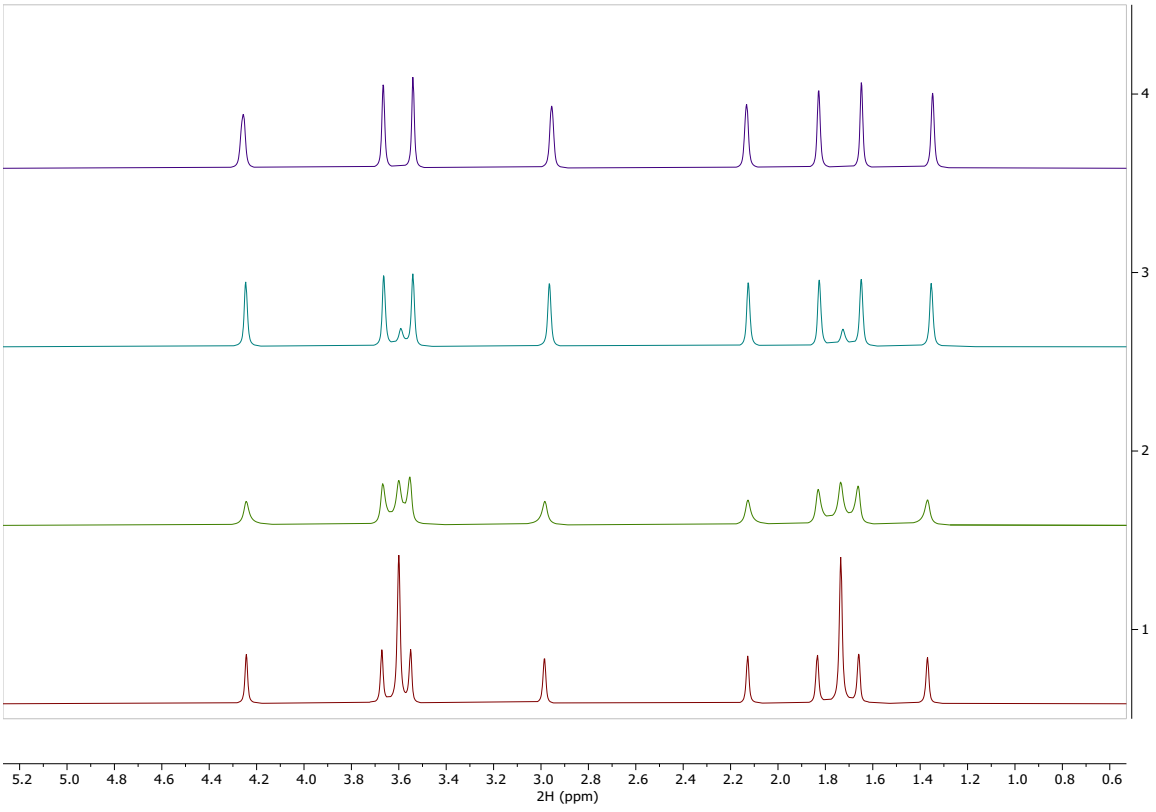


Figure S3. ^{2}H RQC spectra with 11.3 %, 11.5%, 11.8%, and 12.1% (w/v) PBLG in THF-d_8. Alignment is fully achieved at 12.1% PBLG

RCSA Experimental Procedure

Sample Preparation

Parthenolide: 10.16 mg of parthenolide (A2B Chem, CA) was dissolved in 600 µL of THF-d_8 with 10 µL of tetramethylsilane (TMS) for chemical shift referencing. For RCSA measurements, three ^{13}C NMR spectra were acquired without PBLG, with 31.99 mg PBLG and with a total of 88.87 mg PBLG. The chemical shift difference obtained in the first two ^{13}C spectra corresponds to two isotropic states at different concentration, and it was extrapolated to compensated for the chemical shift changes due to the addition of PBLG at the highest PBLG concentration in mesophase. For the RCSA measurement conducted in $CDCl_3$, 9.66 mg of parthenolide was dissolved in 600 µL of $CDCl_3$ with 10 µL of TMS, and the total amount of PBLG added to the sample were 37.18 mg and 88.73 mg, respectively.

Dexamethasone: A sample of 9.96 mg of dexamethasone (Astatech, PA) was prepared in 600 µL THF-d_8 with successive addition of 0 mg, 28.65 mg, 57.10 mg, 29.88 mg, 42.32 mg, 50.51 mg, and 44.12 mg PBLG. ^{13}C spectra and THF-d_8 RQC were measured at each PBLG concentration.

Sucrose: 7.5 mg sucrose (Oakwood Chemical, SC) was dissolved in a mixture of 480 µL THF-d_8 and 120 µL DMSO-d_6. 10 µL TMS was added for chemical shift referencing. The total amount of PBLG used to acquire the second isotropic and third anisotropic spectra were 31.49 mg and 124.91 mg. The final PBLG concentration is above the critical concentration in order to observe larger ^{13}C RCSAs from sucrose.

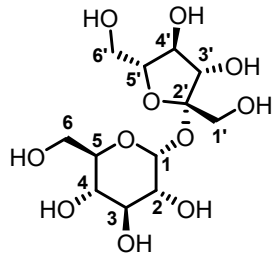
NMR Data Acquisition

All NMR data were collected on a Bruker Avance III 600 MHz spectrometer equipped with a prodigy BBO probe at 15°C. ^{13}C spectra were acquired using standard $^{13}C\{^1H\}$ experiments with an acquisition time of 2.2 s in 1024 scans. RQC was measured from a single scan ^2H spectra with an acquisition time of 2 s.

DFT Calculation

The conformers of parthenolide and dexamethasone, along with their diastereomers, were initially optimized through a conformer search. Geometry optimization was further performed using Density Functional Theory (DFT) in Gaussian at the B3LYP/6-31G(d) level. After optimization, chemical shift tensors were calculated using the mPW1PW91 functional with the 6-311+G(2d,p) basis set, applying the SCRF model with chloroform as the solvent. The chemical shift tensors from the lowest-energy conformer were used in Singular Value Decomposition (SVD) fitting to back-calculate the ^{13}C Residual Chemical Shift Anisotropies (RCSAs).

For the conformers of sucrose and *epi*-sucrose, geometry optimization was conducted at the B3LYP/6-31G(d) level in DMSO and the ^{13}C chemical shift tensors were obtained at wB97XD/def2SVP level. Based on the dihedral angles φ (O5-C1-O-C2') and ψ (C1-O-C2'-O5'), the conformers of sucrose and *epi*-sucrose were classified into four clusters M1-M4, respectively (Figure S4 and S5). Both sucrose and *epi*-sucrose exhibited the largest population and included the low-energy conformers. Four conformers with lowest energy in M1 cluster were used for SVD fitting for RCSA calculation.



Structure of sucrose with labels

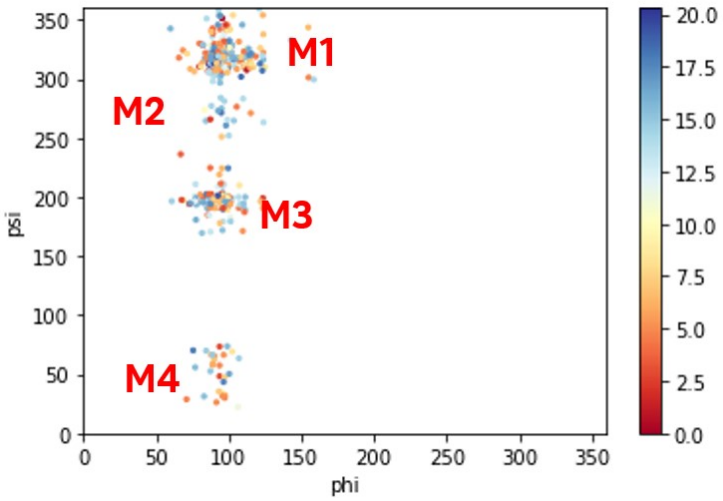


Figure S4. Distribution of sucrose conformers based on dihedral angles φ and ψ, with energy values (kcal/mol) represented using a color-coded scale.

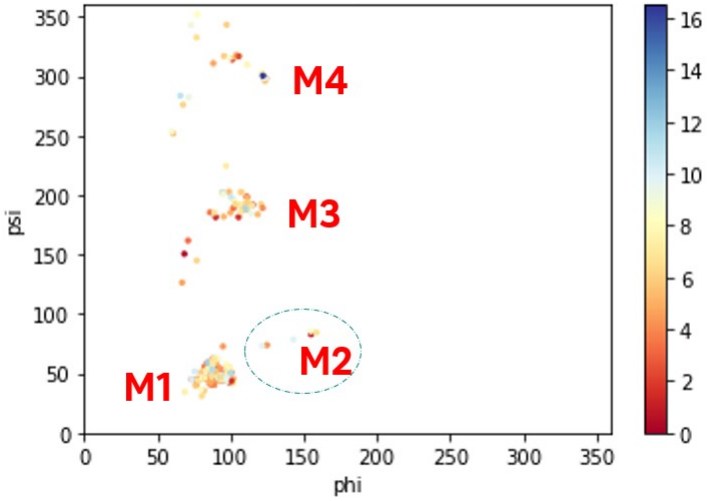


Figure S5. Distribution of 2'-*epi* sucrose conformers based on dihedral angles φ and ψ, with energy values (kcal/mol) represented using a color-coded scale.

Sucrose Solubility

The solubility of sucrose in co-solvent systems was measured by adding over 60 mg sucrose solid to 1 mL of each of the following mixtures: $CDCl_3$/DMSO-d_6 = 80%:20%, $CDCl_3$/DMSO-d_6 = 70%:30%, THF-d_8/DMSO-d_6 = 80%:20%, and THF-d_8/DMSO-d_6 = 70%:30%. After sucrose addition, the samples were stirred overnight at room temperature. Subsequently, the supernatant from each sample was transferred into an NMR tube for 1H NMR analysis. Each ^{1}H spectrum was acquired over 32 scans, with a 30-second interval between acquisitions to ensure complete signal recovery (Figure S6). The solubility of sucrose was determined by comparing the integral of the sucrose peak at 5.35 ppm with the peak of 10.106 mg melatic acid in DMSO-d6, where melatic acid is an external standard for quantitative concentration measurements. Additionally, the signal-to-noise (SNR) ratio of sucrose in the mixture of 600 µL THF-d_8/DMSO-d_6 80%:20% was determined from a 32-scan ^{13}C spectrum (Figure S7).

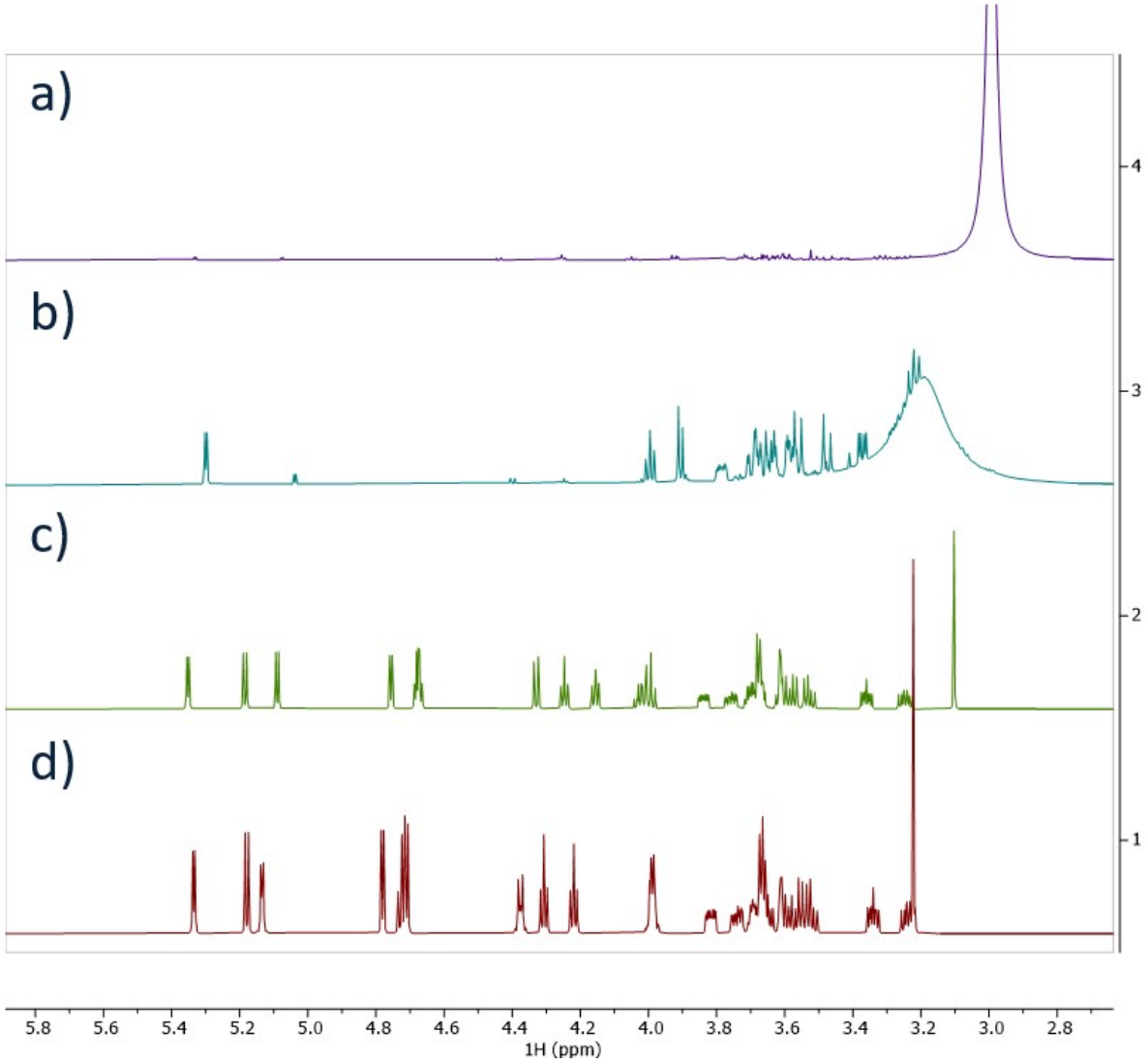


Figure S6. ^{1}H spectra of sucrose in 600 µL a) $CDCl_3$/DMSO-d_6 = 80%:20%, b) $CDCl_3$/DMSO-d_6 = 70%:30%, c) THF-d_8/DMSO-d_6 = 80%:20%, and d) THF-d_8/DMSO-d_6 = 70%:30%. Both a) and b) are scaled up 64-fold.

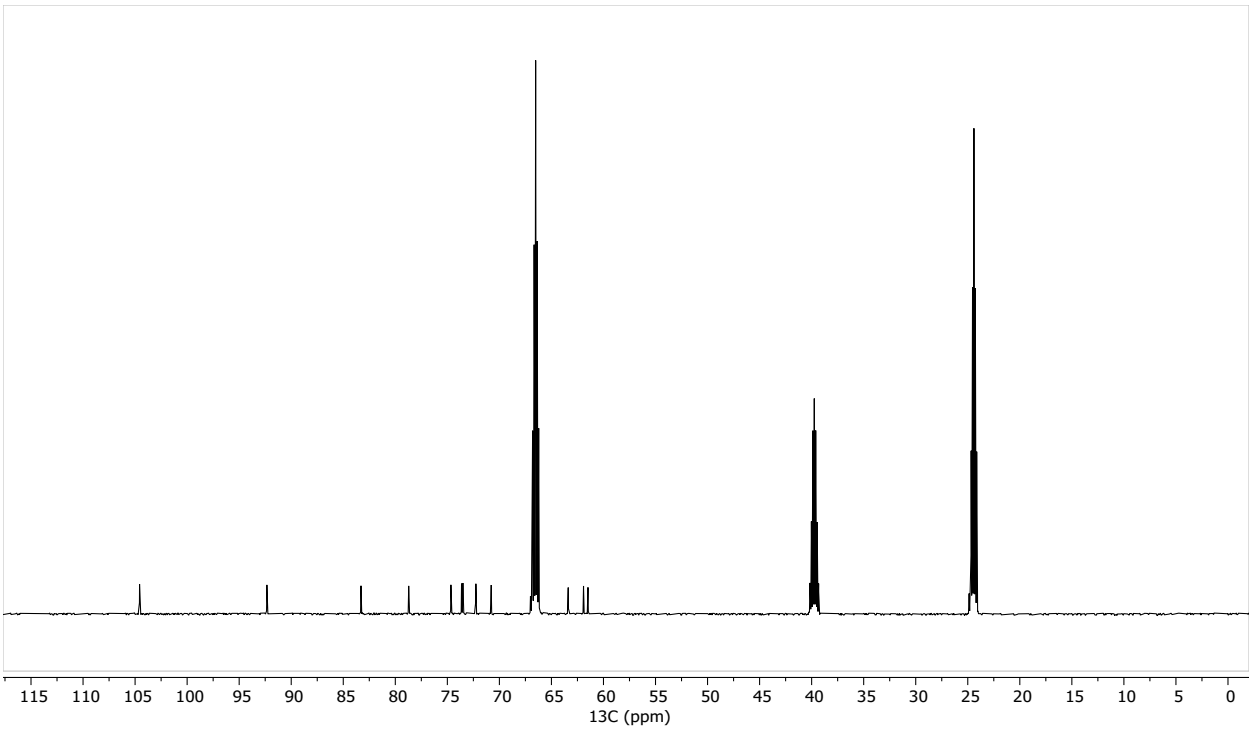


Figure S7. 32-scan ^{13}C spectra of 7.5 mg sucrose in 600 µL THF-d_8/DMSO-d_6 = 80%:20%.

Sucrose RCSA

Given the inherent flexibility of sucrose, relying on a single calculated conformer was insufficient for comprehensive conformational characterization. Following the procedure described in our previous study,[23] over 300 calculated conformers of sucrose were classified into 4 clusters based on their dihedral angles, φ and ψ (Figure S4). Among these, the largest population was found in cluster M1, from which four conformers with the best-fitting *Q*-values were selected to depict the epitope of sucrose. A weighted average *Q*-value from these selected conformers reflected the agreement between experimental and calculated RCSA values for sucrose.

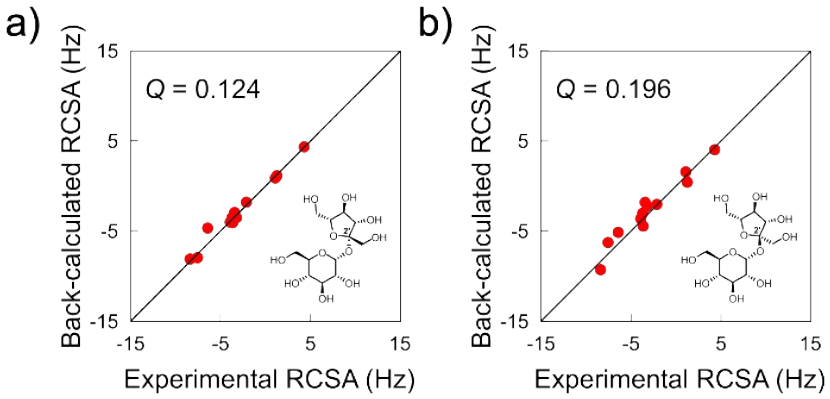


Figure S8. Experimental and back-calculated ^{13}C RCSA plots for a) sucrose and b) 2'-*epi* sucrose based on weighted average analysis of the four lowest-*Q* conformers from DFT calculations.

Alignment in THF-d_8/DMSO-d_6 co-solvent system

As the concentration of DMSO-d_6 increased in the THF-d_8/DMSO-d_6 mixture, the alignment amplitude also increased in the presence of a similar amount of PBLG (Figure S8). However, when the DMSO-d_6 concentration reached 70%, dissolving the same amount of PBLG became very difficult. After plenty of inversions, the sample transformed into a jelly-like homogeneous state. Despite this, full alignment was not achieved due to the limited solubility of PBLG (Figure S9).

In contrast, increasing the concentration of DMSO-d_6 in the $CDCl_3$/ DMSO-d_6 mixture led to a decrease in alignment amplitude (Table 1). The maximum DMSO-d_6 concentration can be used in this system was 30%.

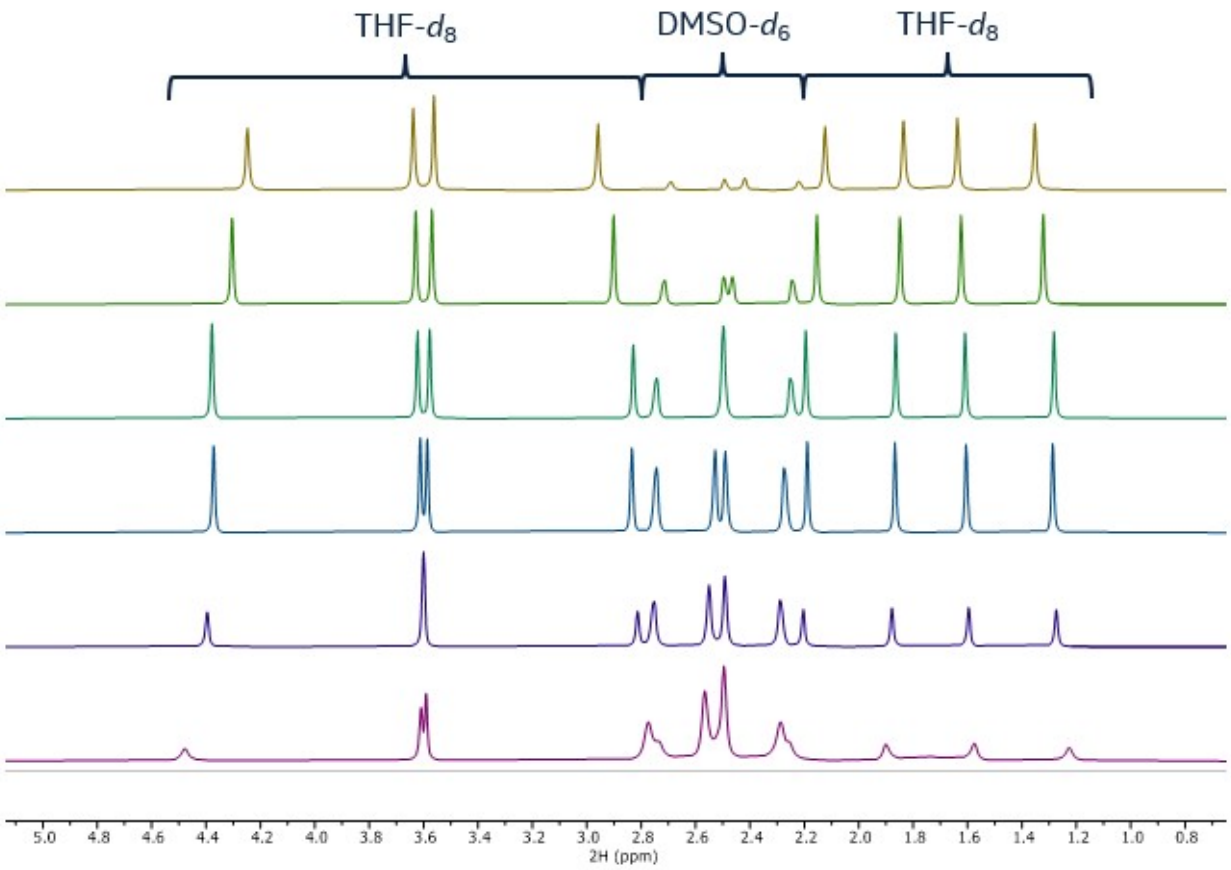


Figure S9. Alignment at varied THF-d_8/DMSO-d_6 volumetric ratio. From top to bottom: ^{2}H RQC spectra with 13.3 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 90%:10%, 13.6 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 80%:20%, 13.8 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 70%:30%, 13.8 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 60%:40%, 13.5 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 50%:50%, 13.8 % (w/v) PBLG in THF-d_8/DMSO-d_6 = 40%:60%.

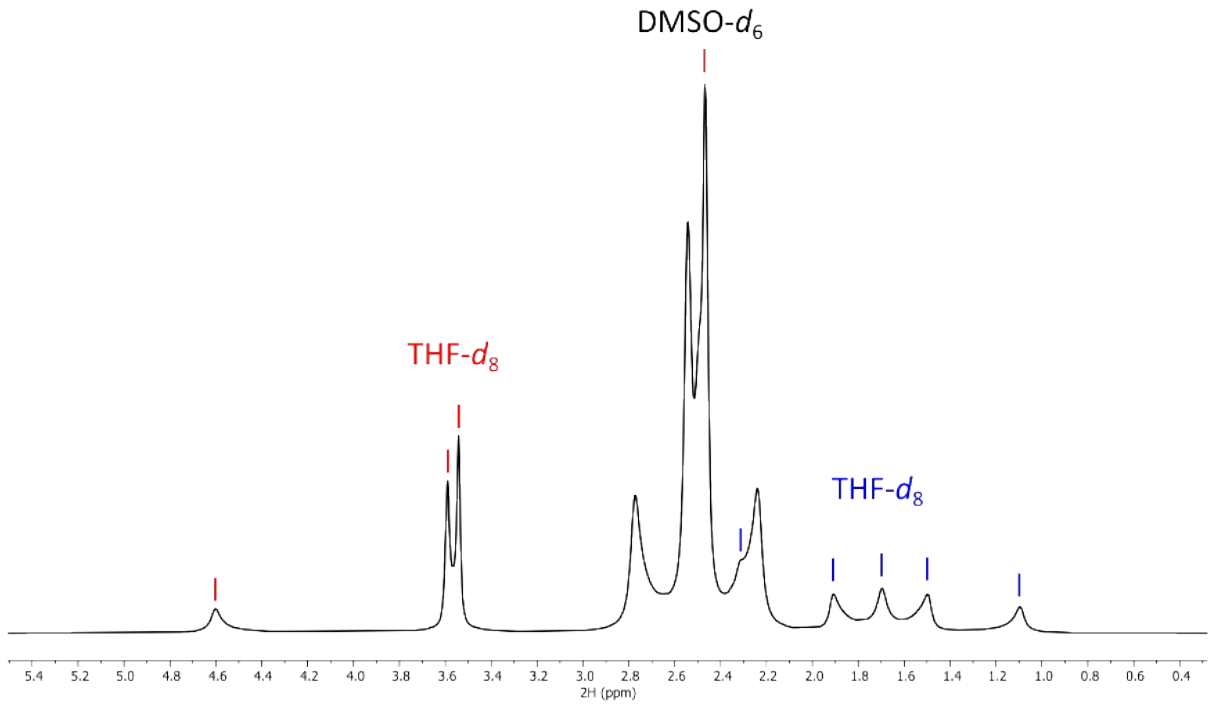


Figure S10. Partially aligned spectrum in THF-d_8/DMSO-d_6 = 30%:70% with 13.7 % (w/v) PBLG.

Table S2. PBLG-induced alignment in $CDCl_3$/DMSO-d_6 solvent system at different volumetric ratio

Solvent	PBLG (% w/v)	Alignment (Hz)
$CDCl_3$/DMSO-d_6 = 90%:10%	13.0	146.83
$CDCl_3$/DMSO-d_6 = 70%:30%	15.2	137.95

When 14.6% PBLG was added to a 60%:40% $CDCl_3$/DMSO-d_6 mixture, alignment was not achieved; however, when the concentration of PBLG increased to 18.3%, PBLG was no longer dissolved in 60%:40% $CDCl_3$/DMSO-d_6.

RCSA Analysis

Parthenolide

Table S3. Parthenolide experimental RCSAs obtained in THF-d_8 and $CDCl_3$ PBLG LLC solutions.

Atom	RCSAs in THF-d_8	RCSAs in $CDCl_3$
C14	-2.24	1.22
C15	4.29	6.14
C8	-5.46	-4.23
C4	-2.84	-4.66
C9	4.43	1.15
C5	-3.33	-0.74
C3	-3.10	-0.99
C10	16.42	10.17
C11	15.21	8.25
C12	-13.09	-13.52
C13	34.61	46.83
C7	3.82	-11.66
C6	5.22	-10.38
C2	29.50	36.07
C1	8.26	2.87

Table S4. Q-values for parthenolide and its diastereomers in THF-d_8 and $CDCl_3$ PBLG LLC solutions.

configurations	Q-factor in THF-d_8	Q-factor in $CDCl_3$
SRRS (parthenolide)	0.0586	0.0426
RRRS	0.3348	0.2638
SSRS	0.3199	0.1872
SRSS	0.3413	0.1547
SRRR	0.6354	0.6728
RSRS	0.6354	0.6729
RRSS	0.2577	0.1383
RRRR	0.2249	0.1639

Table S5. Saupe order matrix from SVD fitting for parthenolide in THF-d_8 and $CDCl_3$ PBLG LLC solutions.

Saupe order matrix (x10^3)	in THF-d_8	in $CDCl_3$
S_{yy}	0.677	0.588
S_{zz}	-1.825	-2.330
S_{xy}	-0.583	-0.614
S_{yz}	-0.705	-0.003
S_{xz}	-1.332	-0.200

Dexamethasone

Table S6. Dexamethasone experimental RCSAs obtained at low and high PBLG concentrations in THF- d_8.

Atom	RCSAs at low PBLG conc.	RCSAs at high PBLG conc.
C18	-2.81	-12.69
C21	0.84	2.27
C22	0.75	2.41
C7	-4.79	-22.91
C6	0.36	0.12
C15	-7.30	-32.26
C8	-1.89	-10.04
C16	8.11	36.14
C12	0.14	-1.72
C14	0.02	-0.36
C10	3.92	16.84
C13	4.90	22.19
C20	-6.05	-27.00
C11	-4.23	-22.77
C17	2.98	11.92
C9	0.79	-1.22
C4	-19.42	-84.37
C2	-25.53	-111.90
C1	-16.47	-72.31
C5	-16.57	-72.69
C3	-5.94	-24.26
C19	-0.61	-3.03

Table S7. Q-values for dexamethasone and its epimers at low and high PBLG concentrations in THF- d_8.

configurations	Q-factor at low PBLG conc.	Q-factor at high PBLG conc.
SRSSSSRR (dexamethasone)	0.0856	0.0749
RRSSSSRR	0.3475	0.3547
SSSSSSRR	0.4457	0.447
SRRSSSRR	0.3885	0.387
SRSRSSRR	0.272	0.2966
SRSSRSRR	0.3924	0.3929
SRSSSRRR	0.3686	0.3708
SRSSSSSR	0.1846	0.178

Table S8. Saupe order matrix from SVD fitting for dexamethasone at low and high PBLG concentrations in THF- d_8.

Saupe order matrix (x10^3)	At low PBLG conc.	At high PBLG conc.
S_{yy}	-2.503	-11.051
S_{zz}	-0.870	-3.755
S_{xy}	-0.230	-0.993
S_{yz}	-1.344	-6.254
S_{xz}	-1.510	-6.849

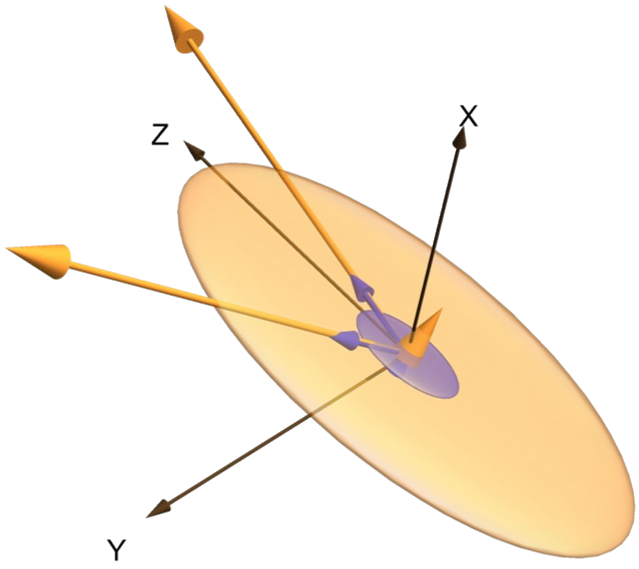


Figure S11. 3D view of principal axis frames for dexamethasone obtained at low (blue) and high (orange) PBLG concentrations in THF- d_8.

Sucrose

Table S9. Sucrose experimental RCSAs obtained in a mixture of THF-d_8/DMSO-d_6 = 80%:20% in PBLG LLC solutions.

Atom	RCSAs
C6	-7.60
C6’	-2.17
C1’	-8.43
C4	4.25
C2	-3.75
C3	-6.47
C5	1.04
C4’	-3.28
C3’	1.22
C5’	-3.97
C1	-3.69
C2’	-3.48

Table S10. Four lowest-Q conformers of sucrose in the M1 cluster and their respective percentage distribution as determined by average weighted fitting.

.out	Q	%
137	0.1943	0.44
235	0.2002	0
355	0.2073	0.36
1	0.2308	0.21
Averaged Q	0.1239	

Table S11. Four lowest-Q conformers of *epi*-sucrose in the M1 cluster and their respective percentage distribution as determined by average weighted fitting.

.out	Q	%
284	0.2494	30
38	0.2981	0
286	0.3002	29
289	0.3093	40
Averaged Q	0.1959	

Structure Coordinates and Chemical Shielding Tensors from DFT computation

Parthenolide

Energy for the lowest-energy conformer: -808.875

The coordinates of the lowest-energy conformer of parthenolide:

C1	-0.23	3.183	-1.977
H2	-0.82	4.107	-1.864
C3	0.873	3.204	-0.87
H4	1.732	2.598	-1.176
C5	-1.101	2.039	-1.5
C6	-2.03	1.324	-2.135
H7	-2.564	0.547	-1.594
H8	-2.289	1.48	-3.178
C9	-0.787	1.787	-0.061
O10	0.29	2.546	0.286
O11	-1.349	1.057	0.717
C12	1.293	4.594	-0.448
H13	0.461	5.302	-0.461
C14	2.652	5.162	-0.595
O15	2.138	4.77	0.694
C16	3.844	4.336	-1.037
H17	4.748	4.726	-0.554
H18	3.997	4.378	-2.119
H19	3.738	3.292	-0.735
C20	2.738	6.658	-0.868
H21	3.66	7.069	-0.437
H22	1.903	7.148	-0.353
C23	2.685	6.982	-2.389
H24	2.567	8.068	-2.503
H25	3.643	6.726	-2.852
C26	1.546	6.249	-3.048
H27	0.559	6.53	-2.674
C28	1.6	5.215	-3.903
C29	2.852	4.72	-4.589
H30	3.746	5.289	-4.324
H31	2.731	4.789	-5.679
H32	3.049	3.663	-4.369
C33	0.349	4.424	-4.227
H34	0.33	4.188	-5.3
H35	-0.545	5.028	-4.024
C36	0.223	3.082	-3.455

H37	1.162	2.517	-3.516
H38	-0.517	2.476	-3.988

SCF GIAO Magnetic shielding tensor (ppm) of the lowest-energy conformer of parthenolide:

1 C Isotropic = 134.4393 Anisotropy = 9.3604

XX= 138.2542 YX= -2.9277 ZX= -4.4894

XY= -1.2686 YY= 134.2329 ZY= -1.0070

XZ= -5.1954 YZ= -5.5425 ZZ= 130.8309

Eigenvalues: 126.5048 136.1336 140.6796

2 H Isotropic = 28.9352 Anisotropy = 2.4299

XX= 29.3575 YX= 0.3053 ZX= -0.8468

XY= 0.5866 YY= 27.2895 ZY= 0.1660

XZ= 2.2249 YZ= -0.6451 ZZ= 30.1587

Eigenvalues: 27.1482 29.1023 30.5552

3 C Isotropic = 100.8668 Anisotropy = 50.8128

XX= 115.3816 YX= -14.5075 ZX= -5.3974

XY= -24.7237 YY= 113.5323 ZY= 3.6620

XZ= -7.5860 YZ= 0.9190 ZZ= 73.6865

Eigenvalues: 72.6845 95.1739 134.7420

4 H Isotropic = 27.9013 Anisotropy = 3.9925

XX= 29.9355 YX= -0.2097 ZX= -1.0410

XY= -0.5603 YY= 26.0084 ZY= 0.3113

XZ= -1.5209 YZ= -0.0825 ZZ= 27.7601

Eigenvalues: 25.9709 27.1701 30.5630

5 C Isotropic = 38.2132 Anisotropy = 136.2966

XX= 2.2726 YX= 55.4909 ZX= -13.8604

XY= 56.7346 YY= -12.9087 ZY= 16.9516

XZ= -13.6901 YZ= 28.1100 ZZ= 125.2755

Eigenvalues: -65.4967 51.0587 129.0776

6 C Isotropic = 58.1248 Anisotropy = 179.3304

XX= -4.6708 YX= 53.4042 ZX= -16.9035

XY= 52.9156 YY= 5.0224 ZY= 18.5743

XZ= -24.5929 YZ= 22.0524 ZZ= 174.0229

Eigenvalues: -56.8521 53.5482 177.6784

7 H Isotropic = 25.0518 Anisotropy = 5.4035

XX= 25.5556 YX= 2.2147 ZX= -0.5318

XY= 3.7297 YY= 25.7308 ZY= 0.1317

XZ= -0.9256 YZ= 0.1111 ZZ= 23.8690

Eigenvalues: 22.4115 24.0897 28.6541

8 H Isotropic = 25.7951 Anisotropy = 7.7065

XX= 29.0615 YX= 4.8547 ZX= -1.0303

XY= 2.1005 YY= 24.2767 ZY= 0.0381

XZ= -0.5210 YZ= 0.5924 ZZ= 24.0470

Eigenvalues: 22.2197 24.2328 30.9328

9 C Isotropic = 10.0298 Anisotropy = 66.5264

XX= 28.2615 YX= -57.0032 ZX= 10.9092

XY= -40.0783 YY= -43.7594 ZY= 15.8813

XZ= 13.5578 YZ= 19.7306 ZZ= 45.5872

Eigenvalues: -72.0845 47.7932 54.3807

10 O Isotropic = 85.0841 Anisotropy = 179.5152

XX= 17.8938 YX= 178.6978 ZX= 4.9845

XY= 128.0443 YY= 74.2210 ZY= -2.6966

XZ= -23.5901 YZ= -9.7339 ZZ= 163.1374

Eigenvalues: -109.9149 160.4062 204.7609

11 O Isotropic = -36.0286 Anisotropy = 541.1040

XX= -264.8811 YX= -10.2117 ZX= 41.7804

XY= -7.4044 YY= -154.0220 ZY= 69.4594

XZ= 62.3251 YZ= 65.4877 ZZ= 310.8172

Eigenvalues: -271.5410 -161.2523 324.7073

12 C Isotropic = 117.2709 Anisotropy = 57.1653

XX= 101.7085 YX= -1.9626 ZX= 31.6390

XY= -5.6281 YY= 114.6911 ZY= -1.6538

XZ= 33.6534 YZ= 10.5106 ZZ= 135.4130

Eigenvalues: 80.9101 115.5214 155.3811

13 H Isotropic = 29.0565 Anisotropy = 5.0485

XX= 27.2296 YX= 2.0392 ZX= 3.0350

XY= 2.4072 YY= 28.1982 ZY= -0.5816

XZ= -0.4890 YZ= -2.7039 ZZ= 31.7418

Eigenvalues: 24.8421 29.9053 32.4222

14 C Isotropic = 120.9573 Anisotropy = 54.5748

XX= 87.2211 YX= -13.9425 ZX= 34.7478

XY= -14.7614 YY= 134.0647 ZY= 14.8986

XZ= 29.7128 YZ= 7.0389 ZZ= 141.5860

Eigenvalues: 67.5517 137.9797 157.3405

15 O Isotropic = 256.4314 Anisotropy = 152.5739

XX= 312.3161 YX= 31.8621 ZX= 5.6963

XY= 44.8227 YY= 101.9266 ZY= 14.6448

XZ= 11.8801 YZ= 6.2142 ZZ= 355.0516

Eigenvalues: 94.8624 316.2845 358.1473

16 C Isotropic = 168.8801 Anisotropy = 30.3356

XX= 162.6278 YX= -2.4830 ZX= -5.0987

XY= 0.5233 YY= 155.3582 ZY= 1.3631

XZ= -0.8514 YZ= 2.3601 ZZ= 188.6542

Eigenvalues: 155.1626 162.3738 189.1038

17 H Isotropic = 30.3775 Anisotropy = 10.0394

XX= 29.8588 YX= 3.4332 ZX= -2.1809

XY= 3.6387 YY= 30.5245 ZY= -3.0280

XZ= -4.0224 YZ= -3.7283 ZZ= 30.7490

Eigenvalues: 26.6397 27.4223 37.0704

18 H Isotropic = 30.2221 Anisotropy = 8.1816

XX= 27.2359 YX= -3.4619 ZX= -0.9739

XY= -2.9293 YY= 33.5439 ZY= 0.9465

XZ= -2.9003 YZ= 2.0287 ZZ= 29.8866

Eigenvalues: 25.5210 29.4688 35.6765

19 H Isotropic = 31.0122 Anisotropy = 8.3057

XX= 31.3918 YX= 0.1082 ZX= 2.6375

XY= 0.2862 YY= 26.7566 ZY= -1.5435

XZ= 2.7069 YZ= -1.9520 ZZ= 34.8882

Eigenvalues: 26.2745 30.2127 36.5494

20 C Isotropic = 147.2260 Anisotropy = 32.2378

XX= 152.2667 YX= -8.6564 ZX= 18.5630

XY= -3.0780 YY= 136.1730 ZY= 0.9220

XZ= 12.6879 YZ= 1.4053 ZZ= 153.2383

Eigenvalues: 131.4431 141.5170 168.7179

21 H Isotropic = 29.6368 Anisotropy = 8.3135

XX= 31.1244 YX= 3.4543 ZX= 0.3269

XY= 4.0076 YY= 31.6744 ZY= -0.3908

XZ= 1.7346 YZ= 0.0835 ZZ= 26.1117

Eigenvalues: 25.6979 28.0334 35.1791

22 H Isotropic = 30.4824 Anisotropy = 8.2121

XX= 28.7223 YX= -0.5976 ZX= 1.8579

XY= -0.3420 YY= 28.5181 ZY= 3.4722

XZ= 2.2379 YZ= 2.6837 ZZ= 34.2068

Eigenvalues: 26.3950 29.0951 35.9571

23 C Isotropic = 159.1793 Anisotropy = 18.3870

XX= 164.9118 YX= -0.2959 ZX= -0.2100

XY= -0.0634 YY= 168.6317 ZY= -8.5908

XZ= 5.9007 YZ= -8.3852 ZZ= 143.9944

Eigenvalues: 141.0555 165.0451 171.4373

24 H Isotropic = 29.4784 Anisotropy = 10.8271

XX= 32.2716 YX= -0.4637 ZX= 5.9036

XY= -1.1325 YY= 27.1151 ZY= -1.0633

XZ= 5.4494 YZ= -0.6048 ZZ= 29.0487

Eigenvalues: 24.7443 26.9945 36.6965

25 H Isotropic = 29.1852 Anisotropy = 5.4401

XX= 31.1027 YX= -1.1710 ZX= -3.2021

XY= -0.3499 YY= 28.7667 ZY= 1.4737

XZ= -1.3191 YZ= 2.1422 ZZ= 27.6861

Eigenvalues: 25.9082 28.8355 32.8119

26 C Isotropic = 54.2429 Anisotropy = 130.3153

XX= 39.4182 YX= -53.8529 ZX= 70.4910

XY= -39.5646 YY= 104.2514 ZY= -1.8543

XZ= 67.4353 YZ= -2.9411 ZZ= 19.0592

Eigenvalues: -46.3089 67.9179 141.1198

27 H Isotropic = 26.1234 Anisotropy = 3.7055

XX= 25.8723 YX= 1.5613 ZX= 3.1827

XY= 1.4602 YY= 27.2396 ZY= -0.5177

XZ= 2.1380 YZ= -1.2050 ZZ= 25.2584

Eigenvalues: 22.3283 27.4482 28.5938

28 C Isotropic = 41.5327 Anisotropy = 171.2292

XX= 20.3673 YX= -60.5987 ZX= 79.5718

XY= -67.3099 YY= 89.8354 ZY= -13.8137

XZ= 82.2368 YZ= -24.7796 ZZ= 14.3954

Eigenvalues: -70.2579 39.1706 155.6855

29 C Isotropic = 168.8791 Anisotropy = 23.4748

XX= 163.5542 YX= -7.5966 ZX= -11.1720

XY= -9.6195 YY= 170.4416 ZY= 0.6985

XZ= -15.8219 YZ= -0.1493 ZZ= 172.6415

Eigenvalues: 151.3008 170.8076 184.5290

30 H Isotropic = 29.5170 Anisotropy = 5.3493

XX= 31.1699 YX= 2.3962 ZX= -1.9760

XY= 1.3768 YY= 29.6816 ZY= 2.6343

XZ= -3.8708 YZ= 0.7529 ZZ= 27.6994

Eigenvalues: 24.8242 30.6436 33.0832

31 H Isotropic = 30.3358 Anisotropy = 10.9715

XX= 28.7911 YX= -4.1147 ZX= -2.3675

XY= -3.3018 YY= 35.3585 ZY= 1.9246

XZ= -1.4923 YZ= 1.9987 ZZ= 26.8579

Eigenvalues: 25.6523 27.7050 37.6502

32 H Isotropic = 30.0020 Anisotropy = 4.8945

XX= 29.5793 YX= -0.5535 ZX= 1.0162

XY= -1.1123 YY= 27.5542 ZY= -0.3646

XZ= 1.3861 YZ= 0.7596 ZZ= 32.8725

Eigenvalues: 27.1892 29.5518 33.2650

33 C Isotropic = 142.3120 Anisotropy = 21.3412

XX= 152.2533 YX= 5.1011 ZX= -7.7730

XY= 5.1862 YY= 137.0232 ZY= -6.7858

XZ= -5.0707 YZ= -0.0308 ZZ= 137.6595

Eigenvalues: 133.8864 136.5101 156.5395

34 H Isotropic = 29.2999 Anisotropy = 7.9892

XX= 28.6466 YX= -1.1471 ZX= -0.0120

XY= -0.7606 YY= 34.4738 ZY= 0.3664

XZ= -0.8913 YZ= -0.5586 ZZ= 24.7794

Eigenvalues: 24.7230 28.5508 34.6260

35 H Isotropic = 29.5165 Anisotropy = 5.8435

XX= 28.6831 YX= 0.2523 ZX= -0.0699

XY= 1.0941 YY= 28.5382 ZY= -3.9590

XZ= 0.5170 YZ= -2.3996 ZZ= 31.3282

Eigenvalues: 26.2663 28.8711 33.4121

36 C Isotropic = 152.0911 Anisotropy = 25.4487

XX= 157.6491 YX= -8.9180 ZX= 2.1150

XY= -9.5381 YY= 159.8668 ZY= 9.4956

XZ= 4.2528 YZ= 9.9022 ZZ= 138.7574

Eigenvalues: 133.2133 154.0031 169.0569

37 H Isotropic = 29.9702 Anisotropy = 4.6892

XX= 29.6359 YX= -0.8401 ZX= -0.1667

XY= -0.8669 YY= 28.0844 ZY= 1.4501

XZ= -1.6394 YZ= 1.6930 ZZ= 32.1901

Eigenvalues: 27.4161 29.3981 33.0963

38 H Isotropic = 29.6570 Anisotropy = 9.2290

XX= 33.6416 YX= 2.4870 ZX= 0.8030

XY= 2.7121 YY= 32.1235 ZY= 0.9352

XZ= 1.0893 YZ= 2.0638 ZZ= 23.2058

Eigenvalues: 22.9338 30.2275 35.8096

Dexamethasone

Energy for the lowest-energy conformer: -1331.197

The coordinates of the lowest-energy conformer of dexamethasone:

C1	0.421	-5.15	-7.083
C2	0.774	-3.887	-7.764
C3	0.732	-2.708	-7.13
O4	0.468	-6.235	-7.658
C5	-0.001	-5.026	-5.676
C6	-0.054	-3.852	-5.022
C7	-0.448	-3.758	-3.571
C8	0.648	-3.062	-2.744
C9	1.111	-1.722	-3.35
C10	2.335	-1.181	-2.594
C11	2.257	-0.958	-1.074
C12	3.447	0.004	-0.752
C13	4.446	-0.558	0.264
C14	4.095	0.365	-2.136
O15	5.213	-0.465	-2.464
C16	4.664	1.783	-2.154
O17	4.113	2.709	-1.578
C18	5.951	2.062	-2.921
O19	6.233	3.435	-2.945
C20	2.891	0.155	-3.152
C21	1.876	1.314	-3.038
C22	3.305	-0.078	-4.613
C23	2.18	-0.671	-5.491
O24	1.182	0.293	-5.829
C25	1.481	-1.9	-4.847
F26	2.51	-2.879	-4.874
C27	0.3	-2.529	-5.694
C28	-0.984	-1.641	-5.729
H29	0.292	-0.996	-3.286
H30	3.114	-1.939	-2.768
H31	1.058	-3.968	-8.81
H32	0.959	-1.791	-7.67
H33	-0.267	-5.957	-5.181
H34	-0.642	-4.759	-3.171
H35	-1.387	-3.195	-3.475
H36	0.288	-2.895	-1.722
H37	1.513	-3.732	-2.675
H38	1.301	-0.504	-0.788

H39	2.339	-1.898	-0.518
H40	3.055	0.942	-0.349
H41	5.277	0.135	0.437
H42	3.946	-0.729	1.224
H43	4.875	-1.513	-0.06
H44	4.938	-1.393	-2.423
H45	6.758	1.484	-2.442
H46	5.861	1.662	-3.942
H47	5.575	3.843	-2.348
H48	0.973	1.096	-3.611
H49	1.592	1.526	-2.005
H50	2.301	2.238	-3.442
H51	4.156	-0.766	-4.644
H52	3.647	0.853	-5.09
H53	2.652	-1.047	-6.41
H54	1.638	1.097	-6.122
H55	-1.785	-2.208	-6.213
H56	-1.324	-1.361	-4.728
H57	-0.806	-0.724	-6.289

SCF GIAO Magnetic shielding tensor (ppm) of the lowest-energy conformer of dexamethasone:

1 C Isotropic = -4.1436 Anisotropy = 172.5518

XX= 15.7018 YX= -14.7335 ZX= 68.3786

XY= -12.9198 YY= -85.1145 ZY= -18.5695

XZ= 69.4964 YZ= -17.0010 ZZ= 56.9818

Eigenvalues: -87.7067 -35.6151 110.8909

2 C Isotropic = 49.6823 Anisotropy = 137.4533

XX= 85.8484 YX= 1.7906 ZX= 40.2625

XY= 7.2234 YY= -45.1268 ZY= -27.1213

XZ= 41.9007 YZ= -23.2643 ZZ= 108.3254

Eigenvalues: -50.1055 57.8346 141.3179

3 C Isotropic = 25.6159 Anisotropy = 187.2657

XX= 58.7821 YX= -45.8844 ZX= 56.7418

XY= -28.1474 YY= -91.0599 ZY= -2.3158

XZ= 62.8658 YZ= 4.7290 ZZ= 109.1254

Eigenvalues: -100.8544 27.2422 150.4597

4 O Isotropic = -219.7532 Anisotropy = 846.8820

XX= -351.9233 YX= -55.9812 ZX= 499.6693

XY= -57.3099 YY= -281.4638 ZY= -47.5169

XZ= 498.8981 YZ= -50.6158 ZZ= -25.8724

Eigenvalues: -714.8010 -289.2933 344.8348

5 C Isotropic = 54.7056 Anisotropy = 110.8406

XX= 84.9530 YX= -24.6892 ZX= 29.4823

XY= -23.5922 YY= -26.6759 ZY= -4.3328

XZ= 29.6541 YZ= -2.3173 ZZ= 105.8397

Eigenvalues: -31.7303 67.2478 128.5994

6 C Isotropic = 10.1783 Anisotropy = 214.6128

XX= 42.9879 YX= 10.8401 ZX= 80.0473

XY= -15.6460 YY= -101.0270 ZY= -25.8224

XZ= 82.7627 YZ= -38.8845 ZZ= 88.5739

Eigenvalues: -107.4124 -15.3062 153.2535

7 C Isotropic = 152.0184 Anisotropy = 17.4275

XX= 155.3472 YX= -2.5413 ZX= 0.5856

XY= -8.3830 YY= 159.4415 ZY= 7.5402

XZ= -0.9675 YZ= -0.4898 ZZ= 141.2663

Eigenvalues: 140.5563 151.8621 163.6367

8 C Isotropic = 155.2290 Anisotropy = 26.8976

XX= 170.4657 YX= 3.3959 ZX= 4.4362

XY= 9.6877 YY= 155.2995 ZY= -3.2255

XZ= 5.2361 YZ= -6.2990 ZZ= 139.9219

Eigenvalues: 137.2666 155.2597 173.1608

9 C Isotropic = 147.6646 Anisotropy = 14.2970

XX= 155.8802 YX= -6.6450 ZX= -2.2983

XY= -0.5793 YY= 146.6805 ZY= 6.3752

XZ= 6.0000 YZ= -2.0364 ZZ= 140.4329

Eigenvalues: 139.2349 146.5629 157.1959

10 C Isotropic = 137.5054 Anisotropy = 36.2199

XX= 151.0932 YX= 13.1990 ZX= 8.6632

XY= 4.5599 YY= 152.9191 ZY= 2.8436

XZ= -1.4482 YZ= 7.3008 ZZ= 108.5038

Eigenvalues: 107.7701 143.0940 161.6520

11 C Isotropic = 152.5038 Anisotropy = 41.9028

XX= 177.0744 YX= -5.1860 ZX= 12.1045

XY= -3.7198 YY= 151.9427 ZY= -0.7259

XZ= 11.6736 YZ= 2.2252 ZZ= 128.4944

Eigenvalues: 125.6251 151.4474 180.4390

12 C Isotropic = 143.1039 Anisotropy = 37.5845

XX= 143.4303 YX= -0.4174 ZX= 12.4478

XY= -3.0628 YY= 163.7170 ZY= 13.7161

XZ= 3.9319 YZ= 14.7874 ZZ= 122.1645

Eigenvalues: 115.2760 145.8756 168.1602

13 C Isotropic = 171.0560 Anisotropy = 23.3033

XX= 177.2764 YX= -2.7929 ZX= 10.4660

XY= -4.8936 YY= 170.2466 ZY= -9.4994

XZ= 10.2431 YZ= -5.5594 ZZ= 165.6450

Eigenvalues: 157.6333 168.9433 186.5915

14 C Isotropic = 89.0344 Anisotropy = 16.6252

XX= 87.4219 YX= -3.2665 ZX= 5.4597

XY= -10.3743 YY= 95.5138 ZY= -2.3954

XZ= 2.4617 YZ= -0.7879 ZZ= 84.1676

Eigenvalues: 80.8965 86.0889 100.1179

15 O Isotropic = 281.4040 Anisotropy = 66.3610

XX= 301.9906 YX= 22.7748 ZX= -41.6810

XY= 34.7957 YY= 288.5796 ZY= 23.5009

XZ= -2.6871 YZ= 10.0758 ZZ= 253.6417

Eigenvalues: 231.7579 286.8094 325.6446

16 C Isotropic = -38.2253 Anisotropy = 198.6924

XX= -38.3318 YX= -83.7532 ZX= 46.7856

XY= -90.2952 YY= -14.8428 ZY= -43.2689

XZ= 47.6274 YZ= -64.6667 ZZ= -61.5013

Eigenvalues: -114.4005 -94.5118 94.2363

17 O Isotropic = -251.3804 Anisotropy = 970.6690

XX= -239.9564 YX= -299.5290 ZX= 413.2315

XY= -285.1024 YY= -22.3585 ZY= -239.1494

XZ= 383.8195 YZ= -244.9853 ZZ= -491.8262

Eigenvalues: -784.6971 -365.1763 395.7323

18 C Isotropic = 114.8803 Anisotropy = 53.8327

XX= 132.8474 YX= 18.1809 ZX= 4.3160

XY= 22.0268 YY= 127.9444 ZY= -14.7049

XZ= 8.9887 YZ= -8.5995 ZZ= 83.8491

Eigenvalues: 78.3238 115.5483 150.7688

19 O Isotropic = 320.1456 Anisotropy = 52.3282

XX= 296.5061 YX= -11.8062 ZX= 3.9372

XY= -12.2149 YY= 327.0626 ZY= 28.8674

XZ= -10.0651 YZ= 12.7296 ZZ= 336.8683

Eigenvalues: 291.9033 313.5025 355.0311

20 C Isotropic = 130.5232 Anisotropy = 31.7918

XX= 138.8809 YX= -2.8954 ZX= 20.4771

XY= -7.0632 YY= 133.6775 ZY= 9.2679

XZ= 19.5645 YZ= -3.5063 ZZ= 119.0112

Eigenvalues: 105.6717 134.1800 151.7177

21 C Isotropic = 168.7722 Anisotropy = 15.0764

XX= 164.3947 YX= -0.1924 ZX= -3.6426

XY= 2.5309 YY= 164.7058 ZY= 1.2711

XZ= -5.9228 YZ= -1.6010 ZZ= 177.2160

Eigenvalues: 162.3325 165.1609 178.8231

22 C Isotropic = 145.9163 Anisotropy = 15.0289

XX= 150.0912 YX= -5.7343 ZX= -2.0261

XY= -1.9393 YY= 153.1757 ZY= -4.2379

XZ= 0.5008 YZ= -1.3000 ZZ= 134.4819

Eigenvalues: 133.9699 147.8434 155.9355

23 C Isotropic = 109.2469 Anisotropy = 48.4303

XX= 98.6180 YX= 4.7362 ZX= -9.4204

XY= 2.2395 YY= 101.5773 ZY= -25.4502

XZ= 0.3480 YZ= -20.1133 ZZ= 127.5453

Eigenvalues: 88.2835 97.9234 141.5338

24 O Isotropic = 260.6065 Anisotropy = 91.8791

XX= 279.5171 YX= 47.3033 ZX= 10.4678

XY= 37.2184 YY= 279.6765 ZY= -32.8053

XZ= 26.4115 YZ= -2.9630 ZZ= 222.6259

Eigenvalues: 203.2627 256.6976 321.8592

25 C Isotropic = 79.7356 Anisotropy = 55.3511

XX= 61.9788 YX= -7.5507 ZX= -3.7141

XY= -5.7725 YY= 64.7130 ZY= -14.7635

XZ= -1.2532 YZ= -14.4688 ZZ= 112.5151

Eigenvalues: 54.1670 68.4035 116.6364

26 F Isotropic = 356.9378 Anisotropy = 22.2808

XX= 355.7076 YX= 17.4305 ZX= -3.3601

XY= 14.4100 YY= 354.1101 ZY= -8.2562

XZ= 9.0049 YZ= -6.2334 ZZ= 360.9957

Eigenvalues: 336.8058 362.2159 371.7917

27 C Isotropic = 132.0149 Anisotropy = 46.6803

XX= 134.5258 YX= -1.7242 ZX= 25.9579

XY= -3.2021 YY= 118.5632 ZY= -4.9264

XZ= 21.6683 YZ= 1.0534 ZZ= 142.9557

Eigenvalues: 114.4519 118.4577 163.1351

28 C Isotropic = 162.5751 Anisotropy = 31.6877

XX= 156.7873 YX= -2.7904 ZX= 9.1551

XY= -0.3029 YY= 150.4179 ZY= -6.7708

XZ= 5.0680 YZ= -5.5548 ZZ= 180.5201

Eigenvalues: 149.2015 154.8235 183.7002

29 H Isotropic = 29.1547 Anisotropy = 3.0604

XX= 31.0103 YX= 0.5452 ZX= 0.0844

XY= 0.5741 YY= 26.3937 ZY= -0.5851

XZ= 0.7700 YZ= -0.6542 ZZ= 30.0602

Eigenvalues: 26.2108 30.0584 31.1950

30 H Isotropic = 29.9023 Anisotropy = 6.1160

XX= 33.8573 YX= -0.8293 ZX= 0.1724

XY= -0.8564 YY= 27.1105 ZY= -0.2978

XZ= 0.3472 YZ= -0.5853 ZZ= 28.7391

Eigenvalues: 26.9155 28.8118 33.9797

31 H Isotropic = 25.1233 Anisotropy = 5.9636

XX= 27.7081 YX= 0.2629 ZX= -2.4659

XY= 0.0698 YY= 22.8421 ZY= -0.3845

XZ= -2.3535 YZ= -0.6565 ZZ= 24.8197

Eigenvalues: 22.6467 23.6241 29.0991

32 H Isotropic = 24.0216 Anisotropy = 10.0182

XX= 26.5934 YX= -4.9783 ZX= -1.5489

XY= -4.2307 YY= 23.0150 ZY= 2.3504

XZ= -1.6249 YZ= 2.8673 ZZ= 22.4565

Eigenvalues: 19.2298 22.1346 30.7004

33 H Isotropic = 25.3213 Anisotropy = 7.2081

XX= 28.3987 YX= -0.8796 ZX= -2.9417

XY= -0.7889 YY= 22.6435 ZY= 0.8196

XZ= -2.6405 YZ= 0.9280 ZZ= 24.9216

Eigenvalues: 22.3433 23.4939 30.1267

34 H Isotropic = 29.3273 Anisotropy = 10.0909

XX= 31.8754 YX= 3.9211 ZX= -1.4509

XY= 4.4529 YY= 31.5004 ZY= -0.8456

XZ= -1.2312 YZ= -0.4470 ZZ= 24.6061

Eigenvalues: 24.3646 27.5628 36.0546

35 H Isotropic = 28.9282 Anisotropy = 6.8460

XX= 27.5293 YX= 1.8831 ZX= 3.4433

XY= 0.9669 YY= 28.2447 ZY= 2.1795

XZ= 1.6926 YZ= 1.7896 ZZ= 31.0106

Eigenvalues: 26.0797 27.2126 33.4922

36 H Isotropic = 29.8228 Anisotropy = 7.5262

XX= 32.1681 YX= -1.2375 ZX= -0.6061

XY= -0.8330 YY= 33.6610 ZY= 3.3439

XZ= 0.4961 YZ= 2.5179 ZZ= 23.6394

Eigenvalues: 22.8401 31.7881 34.8403

37 H Isotropic = 30.1490 Anisotropy = 5.5708

XX= 30.8828 YX= 1.0256 ZX= 0.6086

XY= 1.4846 YY= 29.9173 ZY= -3.7361

XZ= 0.8316 YZ= -4.3031 ZZ= 29.6470

Eigenvalues: 25.4062 31.1780 33.8629

38 H Isotropic = 29.8477 Anisotropy = 6.7859

XX= 29.3738 YX= 0.0129 ZX= 0.8216

XY= -0.3591 YY= 28.9613 ZY= 4.1921

XZ= 0.6186 YZ= 3.9907 ZZ= 31.2081

Eigenvalues: 25.7502 29.4213 34.3716

39 H Isotropic = 30.4864 Anisotropy = 7.5336

XX= 31.4817 YX= 0.4753 ZX= 0.5961

XY= 0.4296 YY= 35.1083 ZY= -2.1396

XZ= 1.4338 YZ= -1.8988 ZZ= 24.8691

Eigenvalues: 24.3218 31.6286 35.5087

40 H Isotropic = 28.4584 Anisotropy = 6.5725

XX= 29.9293 YX= -1.2541 ZX= -3.2933

XY= -1.0703 YY= 26.6200 ZY= -0.0933

XZ= -3.4733 YZ= -1.2365 ZZ= 28.8257

Eigenvalues: 24.9717 27.5633 32.8400

41 H Isotropic = 31.0450 Anisotropy = 11.2270

XX= 36.6247 YX= -1.1218 ZX= 4.2601

XY= -1.0924 YY= 29.2943 ZY= -1.2962

XZ= 4.3671 YZ= -0.9802 ZZ= 27.2161

Eigenvalues: 25.4206 29.1847 38.5297

42 H Isotropic = 30.7432 Anisotropy = 11.4731

XX= 28.5266 YX= -4.1738 ZX= 0.8206

XY= -3.8345 YY= 36.7209 ZY= 1.4099

XZ= 0.6092 YZ= 0.6136 ZZ= 26.9822

Eigenvalues: 25.8765 27.9612 38.3919

43 H Isotropic = 30.9609 Anisotropy = 7.3054

XX= 28.6624 YX= -1.7016 ZX= -0.6735

XY= -1.1141 YY= 30.9361 ZY= -3.8129

XZ= -1.1568 YZ= -3.2469 ZZ= 33.2842

Eigenvalues: 26.8432 30.2083 35.8312

44 H Isotropic = 30.5733 Anisotropy = 13.3920

XX= 33.1298 YX= 6.5519 ZX= -2.6689

XY= 6.5277 YY= 26.8356 ZY= -5.4077

XZ= -2.0057 YZ= -2.6026 ZZ= 31.7544

Eigenvalues: 22.1796 30.0389 39.5013

45 H Isotropic = 26.9623 Anisotropy = 7.5895

XX= 28.5630 YX= 4.8157 ZX= 1.9718

XY= 3.7961 YY= 25.8894 ZY= -4.8838

XZ= 0.2869 YZ= -1.9434 ZZ= 26.4347

Eigenvalues: 20.6557 28.2093 32.0220

46 H Isotropic = 27.1801 Anisotropy = 9.2344

XX= 32.0709 YX= 2.3018 ZX= -2.1993

XY= 2.9961 YY= 27.2950 ZY= 1.3963

XZ= -0.1016 YZ= -1.0607 ZZ= 22.1743

Eigenvalues: 21.9949 26.2090 33.3364

47 H Isotropic = 28.5562 Anisotropy = 16.8578

XX= 25.6580 YX= 2.1896 ZX= -5.9535

XY= 2.8264 YY= 25.7954 ZY= 7.2635

XZ= -3.5456 YZ= 9.1182 ZZ= 34.2154

Eigenvalues: 17.9136 27.9603 39.7948

48 H Isotropic = 29.7448 Anisotropy = 7.5622

XX= 32.9539 YX= -2.4140 ZX= 1.2220

XY= -2.3355 YY= 25.5967 ZY= -2.4197

XZ= 1.8788 YZ= -1.8218 ZZ= 30.6838

Eigenvalues: 24.4543 29.9938 34.7863

49 H Isotropic = 30.7193 Anisotropy = 8.3409

XX= 29.6860 YX= -2.1238 ZX= -3.2472

XY= -2.8265 YY= 29.1062 ZY= 0.7388

XZ= -3.5706 YZ= 2.0661 ZZ= 33.3657

Eigenvalues: 26.5752 29.3028 36.2799

50 H Isotropic = 31.4501 Anisotropy = 8.4389

XX= 32.8779 YX= 3.4548 ZX= -1.4458

XY= 2.5327 YY= 31.6311 ZY= -3.6115

XZ= -1.4875 YZ= -3.7311 ZZ= 29.8415

Eigenvalues: 26.8530 30.4213 37.0761

51 H Isotropic = 29.2946 Anisotropy = 5.2141

XX= 30.3409 YX= -1.4480 ZX= 1.5341

XY= -1.5724 YY= 26.7680 ZY= 2.0341

XZ= 2.8116 YZ= 1.6999 ZZ= 30.7749

Eigenvalues: 25.0545 30.0586 32.7707

52 H Isotropic = 30.4559 Anisotropy = 8.1374

XX= 31.1278 YX= 1.9010 ZX= 0.8460

XY= 1.3974 YY= 34.8597 ZY= 1.4135

XZ= 2.5414 YZ= 1.6268 ZZ= 25.3803

Eigenvalues: 24.8057 30.6812 35.8808

53 H Isotropic = 27.1947 Anisotropy = 5.4418

XX= 28.7191 YX= -2.1589 ZX= -1.0334

XY= -2.3524 YY= 26.5787 ZY= 0.5818

XZ= -0.8759 YZ= 2.8436 ZZ= 26.2862

Eigenvalues: 24.4720 26.2895 30.8226

54 H Isotropic = 31.2633 Anisotropy = 16.6633

XX= 31.0939 YX= 7.2251 ZX= 0.2592

XY= 7.1168 YY= 36.6408 ZY= -4.1381

XZ= -0.1192 YZ= -4.6963 ZZ= 26.0551

Eigenvalues: 23.1750 28.2426 42.3721

55 H Isotropic = 31.1780 Anisotropy = 11.3113

XX= 34.3717 YX= -0.7944 ZX= 5.6693

XY= -0.5303 YY= 26.8080 ZY= -1.1902

XZ= 4.6002 YZ= -1.0071 ZZ= 32.3544

Eigenvalues: 26.5692 28.2460 38.7189

56 H Isotropic = 29.9232 Anisotropy = 4.7817

XX= 28.2862 YX= -1.8453 ZX= 1.3446

XY= -1.8971 YY= 28.8970 ZY= 0.3879

XZ= -0.6216 YZ= 2.5277 ZZ= 32.5862

Eigenvalues: 26.4457 30.2128 33.1109

57 H Isotropic = 29.3376 Anisotropy = 6.4241

XX= 28.7817 YX= 2.2433 ZX= 2.1723

XY= 2.6124 YY= 30.2458 ZY= -3.0540

XZ= 0.9204 YZ= -4.4741 ZZ= 28.9854

Eigenvalues: 24.1424 30.2501 33.6204

Sucrose

Energy for the sucrose conformer 137: -1297.58

The coordinates of the sucrose 137.out:

H1	-1.617	0.838	0.517
C2	-1.162	1.351	1.364
C3	-1.22	3.438	2.775
C4	-1.181	1.167	3.799
C5	-1.733	2.59	3.934
C6	-1.618	2.815	1.437
H7	-0.121	3.481	2.839
H8	-0.085	1.205	3.844
H9	-2.834	2.558	3.889
H10	-2.712	2.83	1.366
O11	-1.588	0.618	2.512
C12	-1.688	0.215	4.883
H13	-2.708	-0.103	4.618
H14	-1.739	0.77	5.823
O15	-0.832	-0.892	5.128
H16	-0.723	-1.405	4.306
O17	-1.3	3.118	5.181
H18	-1.491	4.071	5.148
O19	-1.77	4.744	2.919
H20	-1.502	5.239	2.126
O21	-1.138	3.576	0.342
H22	-0.179	3.391	0.224
O23	0.248	1.318	1.281
C24	0.874	0.567	0.245
C25	2.232	0.015	0.813
C26	2.265	-1.422	0.24
C27	0.785	-1.808	0.142
H28	3.079	0.596	0.433
H29	2.838	-2.083	0.903
H30	0.64	-2.463	-0.723
C31	1.005	1.441	-1.016
H32	0.027	1.491	-1.501
H33	1.71	0.963	-1.706
O34	1.368	2.791	-0.74
H35	2.247	2.808	-0.327
O36	2.332	0.038	2.215
H37	1.595	-0.511	2.562
O38	2.77	-1.455	-1.093

H39	3.709	-1.207	-1.06
C40	0.146	-2.477	1.363
H41	0.725	-3.356	1.659
H42	-0.866	-2.803	1.101
O43	0.091	-1.604	2.499
H44	-0.575	-0.902	2.314
O45	0.105	-0.564	-0.142

SCF GIAO Magnetic shielding tensor (ppm) of sucrose 137.out:

1 H Isotropic = 26.2578 Anisotropy = 2.6746

XX= 27.2649 YX= 0.1443 ZX= -1.2809

XY= 0.3552 YY= 24.2265 ZY= 1.2606

XZ= -0.0949 YZ= 0.6742 ZZ= 27.2821

Eigenvalues: 23.8893 26.8434 28.0409

2 C Isotropic = 89.0292 Anisotropy = 35.2747

XX= 81.2481 YX= 1.4575 ZX= -22.9162

XY= 8.6839 YY= 111.1142 ZY= -5.5576

XZ= -15.2986 YZ= 3.7609 ZZ= 74.7252

Eigenvalues: 58.4749 96.0670 112.5457

3 C Isotropic = 108.8923 Anisotropy = 28.5606

XX= 116.4736 YX= -7.6260 ZX= -2.4875

XY= -15.0064 YY= 115.2308 ZY= 5.0284

XZ= -0.2036 YZ= 6.4685 ZZ= 94.9727

Eigenvalues: 93.3130 105.4313 127.9327

4 C Isotropic = 104.4984 Anisotropy = 36.3415

XX= 105.3933 YX= 5.9088 ZX= 23.8047

XY= 2.2353 YY= 106.0560 ZY= 2.7908

XZ= 20.8480 YZ= 11.0267 ZZ= 102.0459

Eigenvalues: 81.1077 103.6614 128.7260

5 C Isotropic = 114.2807 Anisotropy = 41.7083

XX= 115.0083 YX= 8.1975 ZX= 22.6708

XY= 2.1787 YY= 106.8319 ZY= 4.2780

XZ= 19.9243 YZ= 11.9292 ZZ= 121.0020

Eigenvalues: 96.2663 104.4896 142.0863

6 C Isotropic = 112.1895 Anisotropy = 34.8498

XX= 110.8983 YX= 7.0479 ZX= 6.1762

XY= 15.1421 YY= 130.2091 ZY= -1.3168

XZ= 1.3809 YZ= -7.6330 ZZ= 95.4612

Eigenvalues: 93.1117 108.0341 135.4228

7 H Isotropic = 28.1365 Anisotropy = 6.8215

XX= 31.7200 YX= -2.4185 ZX= -1.0081

XY= -2.4905 YY= 26.2813 ZY= 0.4609

XZ= 0.2174 YZ= -0.5297 ZZ= 26.4083

Eigenvalues: 25.3094 26.4160 32.6842

8 H Isotropic = 27.7116 Anisotropy = 4.1067

XX= 29.4962 YX= 0.3244 ZX= 1.8903

XY= 1.1972 YY= 26.9588 ZY= 1.4906

XZ= 0.7973 YZ= 1.0148 ZZ= 26.6797

Eigenvalues: 25.4823 27.2031 30.4494

9 H Isotropic = 28.4746 Anisotropy = 2.1672

XX= 29.0600 YX= 0.4537 ZX= 0.2879

XY= 1.4611 YY= 26.8873 ZY= 0.2973

XZ= -1.2335 YZ= -0.4431 ZZ= 29.4764

Eigenvalues: 26.5223 28.9821 29.9194

10 H Isotropic = 28.4391 Anisotropy = 3.4478

XX= 27.1967 YX= 0.8898 ZX= -1.8143

XY= 0.9926 YY= 28.4976 ZY= -0.4132

XZ= -2.1182 YZ= 1.0321 ZZ= 29.6229

Eigenvalues: 25.7537 28.8259 30.7376

11 O Isotropic = 213.9976 Anisotropy = 74.6580

XX= 185.6291 YX= 20.0849 ZX= -26.7772

XY= 17.3617 YY= 248.5155 ZY= -25.2335

XZ= -18.2407 YZ= -10.1243 ZZ= 207.8481

Eigenvalues: 170.9771 207.2461 263.7696

12 C Isotropic = 121.9052 Anisotropy = 52.1711

XX= 126.1619 YX= -22.5031 ZX= -19.5478

XY= -17.4095 YY= 136.4480 ZY= 7.5056

XZ= -13.3040 YZ= 6.8890 ZZ= 103.1056

Eigenvalues: 94.3113 114.7183 156.6859

13 H Isotropic = 28.2248 Anisotropy = 5.3316

XX= 27.9336 YX= 0.0530 ZX= -4.5996

XY= -0.2012 YY= 29.0043 ZY= -0.5192

XZ= -2.9363 YZ= -1.5988 ZZ= 27.7365

Eigenvalues: 23.9347 28.9605 31.7792

14 H Isotropic = 27.9138 Anisotropy = 5.4289

XX= 31.2194 YX= 0.3921 ZX= 2.2121

XY= -0.9517 YY= 29.9616 ZY= 0.2145

XZ= 1.0669 YZ= 1.2478 ZZ= 22.5604

Eigenvalues: 22.1842 30.0241 31.5331

15 O Isotropic = 293.8125 Anisotropy = 29.2546

XX= 309.9478 YX= -3.7961 ZX= -8.1551

XY= 18.6286 YY= 291.9952 ZY= -1.1947

XZ= -2.0778 YZ= 0.9307 ZZ= 279.4945

Eigenvalues: 278.5611 289.5608 313.3156

16 H Isotropic = 28.5591 Anisotropy = 21.9156

XX= 40.4131 YX= 3.5045 ZX= 6.6255

XY= 2.7010 YY= 25.7765 ZY= 3.4396

XZ= 6.5863 YZ= 2.5802 ZZ= 19.4878

Eigenvalues: 17.0703 25.4375 43.1695

17 O Isotropic = 291.8388 Anisotropy = 42.1375

XX= 288.7164 YX= -14.0309 ZX= 10.5735

XY= -21.4097 YY= 287.3953 ZY= -12.5310

XZ= 24.8839 YZ= 2.0000 ZZ= 299.4048

Eigenvalues: 267.4223 288.1637 319.9305

18 H Isotropic = 29.3610 Anisotropy = 17.4643

XX= 33.8172 YX= -6.8758 ZX= 6.7324

XY= -7.0544 YY= 31.4249 ZY= 1.0028

XZ= 6.3318 YZ= -0.1025 ZZ= 22.8409

Eigenvalues: 18.7405 28.3387 41.0038

19 O Isotropic = 295.5803 Anisotropy = 43.9462

XX= 293.6081 YX= -9.1922 ZX= -9.6698

XY= -6.4453 YY= 316.2491 ZY= -1.5743

XZ= -37.7707 YZ= 18.0115 ZZ= 276.8836

Eigenvalues: 260.0055 301.8575 324.8777

20 H Isotropic = 29.2330 Anisotropy = 16.7402

XX= 28.0320 YX= 0.8385 ZX= 1.0896

XY= 0.8767 YY= 40.3067 ZY= -0.8170

XZ= 2.5041 YZ= -0.9279 ZZ= 19.3602

Eigenvalues: 18.9535 28.3523 40.3931

21 O Isotropic = 292.4948 Anisotropy = 61.9423

XX= 298.6456 YX= 32.9548 ZX= -28.7287

XY= 6.9864 YY= 288.5719 ZY= 4.1536

XZ= -38.4211 YZ= -5.3760 ZZ= 290.2668

Eigenvalues: 255.2155 288.4792 333.7896

22 H Isotropic = 27.1707 Anisotropy = 24.1340

XX= 34.7917 YX= 2.1730 ZX= -12.0296

XY= 1.9872 YY= 23.1862 ZY= -2.2579

XZ= -12.7644 YZ= -2.7624 ZZ= 23.5341

Eigenvalues: 15.4174 22.8346 43.2600

23 O Isotropic = 216.1671 Anisotropy = 41.2934

XX= 209.6776 YX= 8.6210 ZX= 7.1787

XY= 14.1460 YY= 210.3162 ZY= -14.6221

XZ= -35.2905 YZ= -9.2812 ZZ= 228.5077

Eigenvalues: 198.4112 206.3942 243.6961

24 C Isotropic = 71.0144 Anisotropy = 27.7913

XX= 80.7666 YX= -6.9824 ZX= 6.2414

XY= -13.7301 YY= 58.2875 ZY= -8.9722

XZ= 0.6993 YZ= -15.6931 ZZ= 73.9891

Eigenvalues: 49.6303 73.8710 89.5419

25 C Isotropic = 103.7602 Anisotropy = 29.3887

XX= 117.9169 YX= 2.7506 ZX= 17.7957

XY= 3.7134 YY= 97.5053 ZY= 18.8061

XZ= 0.2082 YZ= 5.1958 ZZ= 95.8583

Eigenvalues: 84.0345 103.8934 123.3526

26 C Isotropic = 100.2040 Anisotropy = 22.6628

XX= 113.2226 YX= -0.2693 ZX= -0.3758

XY= 7.6904 YY= 96.9107 ZY= -6.3963

XZ= 12.7373 YZ= 2.0511 ZZ= 90.4788

Eigenvalues: 87.8598 97.4396 115.3126

27 C Isotropic = 96.3471 Anisotropy = 49.1784

XX= 100.3570 YX= -20.1970 ZX= -20.4165

XY= -27.3820 YY= 100.4703 ZY= 5.9422

XZ= -10.6367 YZ= 2.6029 ZZ= 88.2139

Eigenvalues: 71.6650 88.2436 129.1327

28 H Isotropic = 28.1416 Anisotropy = 3.8566

XX= 27.5693 YX= 1.5069 ZX= -1.7383

XY= 2.0908 YY= 28.2517 ZY= -0.7149

XZ= -1.0838 YZ= -0.5769 ZZ= 28.6039

Eigenvalues: 25.8748 27.8373 30.7127

29 H Isotropic = 27.5007 Anisotropy = 5.2198

XX= 29.7907 YX= 0.3427 ZX= -2.3936

XY= -0.3192 YY= 27.9150 ZY= 2.9271

XZ= -2.1118 YZ= 1.9686 ZZ= 24.7965

Eigenvalues: 22.8714 28.6503 30.9806

30 H Isotropic = 27.6454 Anisotropy = 6.6835

XX= 30.2181 YX= -0.6157 ZX= 2.8058

XY= -1.7064 YY= 26.2339 ZY= -1.7296

XZ= 2.5592 YZ= -1.0442 ZZ= 26.4842

Eigenvalues: 24.6708 26.1643 32.1011

31 C Isotropic = 118.2567 Anisotropy = 50.8929

XX= 108.9027 YX= -9.6991 ZX= 17.1992

XY= -12.1040 YY= 134.5661 ZY= -19.3966

XZ= 17.1396 YZ= -16.9782 ZZ= 111.3013

Eigenvalues: 92.2376 110.3472 152.1853

32 H Isotropic = 28.3420 Anisotropy = 3.0203

XX= 26.7521 YX= -0.5707 ZX= 2.5474

XY= -0.1643 YY= 29.2202 ZY= 0.4994

XZ= 1.1860 YZ= 1.0940 ZZ= 29.0538

Eigenvalues: 25.5700 29.1005 30.3556

33 H Isotropic = 27.9913 Anisotropy = 5.1207

XX= 31.1940 YX= 0.6536 ZX= 0.8088

XY= -0.8669 YY= 29.5543 ZY= -0.6722

XZ= 1.7109 YZ= -0.2314 ZZ= 23.2256

Eigenvalues: 23.0029 29.5659 31.4051

34 O Isotropic = 293.6839 Anisotropy = 45.9182

XX= 274.4627 YX= 1.1948 ZX= -7.6514

XY= 2.2827 YY= 282.5477 ZY= 13.6427

XZ= 5.3264 YZ= -7.4009 ZZ= 324.0413

Eigenvalues: 274.0409 282.7147 324.2961

35 H Isotropic = 30.2877 Anisotropy = 15.5734

XX= 24.1228 YX= -1.3953 ZX= -3.0010

XY= -2.4073 YY= 26.7831 ZY= -1.8759

XZ= -2.9829 YZ= -1.8764 ZZ= 39.9572

Eigenvalues: 22.4251 27.7680 40.6700

36 O Isotropic = 277.3361 Anisotropy = 12.2181

XX= 275.8504 YX= -9.5743 ZX= -2.8193

XY= 2.7570 YY= 283.3827 ZY= 6.4681

XZ= -16.7953 YZ= -10.2946 ZZ= 272.7752

Eigenvalues: 263.6984 282.8284 285.4815

37 H Isotropic = 26.6608 Anisotropy = 21.2063

XX= 20.4046 YX= 6.1423 ZX= -2.5284

XY= 6.8497 YY= 30.4217 ZY= -8.3180

XZ= -3.3850 YZ= -9.1018 ZZ= 29.1562

Eigenvalues: 17.0120 22.1721 40.7983

38 O Isotropic = 269.6862 Anisotropy = 72.6017

XX= 269.5483 YX= 20.1329 ZX= 1.0980

XY= 31.5621 YY= 248.8587 ZY= -33.1857

XZ= -11.2204 YZ= -38.6882 ZZ= 290.6516

Eigenvalues: 219.7009 271.2703 318.0873

39 H Isotropic = 30.2780 Anisotropy = 17.9315

XX= 31.3985 YX= 5.2349 ZX= -6.6136

XY= 5.5297 YY= 24.9313 ZY= -5.1767

XZ= -6.1547 YZ= -3.7131 ZZ= 34.5044

Eigenvalues: 21.8197 26.7820 42.2324

40 C Isotropic = 121.7211 Anisotropy = 48.0990

XX= 140.6940 YX= 8.5207 ZX= 25.9450

XY= 4.3093 YY= 115.8045 ZY= -2.9548

XZ= 21.2540 YZ= -1.1882 ZZ= 108.6647

Eigenvalues: 95.0142 116.3619 153.7871

41 H Isotropic = 28.2198 Anisotropy = 8.2522

XX= 29.9096 YX= -3.5992 ZX= 0.6612

XY= -2.7057 YY= 30.8020 ZY= -0.7035

XZ= 1.5897 YZ= -0.8681 ZZ= 23.9480

Eigenvalues: 23.7347 27.2036 33.7213

42 H Isotropic = 27.8826 Anisotropy = 8.9393

XX= 27.1688 YX= 0.1075 ZX= 4.1066

XY= 0.4359 YY= 26.0168 ZY= -3.7646

XZ= 2.7850 YZ= -3.5896 ZZ= 30.4620

Eigenvalues: 22.8648 26.9408 33.8421

43 O Isotropic = 288.1220 Anisotropy = 20.8429

XX= 290.9129 YX= -5.4735 ZX= -10.7698

XY= -15.5869 YY= 290.8255 ZY= -4.4424

XZ= -0.4309 YZ= 2.7604 ZZ= 282.6276

Eigenvalues: 276.6148 285.7340 302.0173

44 H Isotropic = 26.2206 Anisotropy = 25.2202

XX= 36.3853 YX= -9.0757 ZX= -4.4425

XY= -8.9302 YY= 25.8145 ZY= 4.9417

XZ= -5.0994 YZ= 3.7173 ZZ= 16.4622

Eigenvalues: 14.6681 20.9597 43.0341

45 O Isotropic = 220.4155 Anisotropy = 101.3974

XX= 199.7771 YX= -47.0828 ZX= -16.4609

XY= -46.7999 YY= 199.5309 ZY= -56.0073

XZ= -3.4651 YZ= -34.2073 ZZ= 261.9386

Eigenvalues: 139.6758 233.5570 288.0138

Energy for the sucrose conformer 235: -1297.6

The coordinates of the sucrose 235.out:

H1	-1.605	1.134	0.489
C2	-1.152	1.543	1.392
C3	-1.199	3.448	3.022
C4	-1.144	1.04	3.773
C5	-1.634	2.461	4.107
C6	-1.662	2.964	1.653
H7	-0.1	3.513	3.018
H8	-0.046	1.014	3.798
H9	-2.729	2.462	4.162
H10	-2.761	2.91	1.664
O11	-1.589	0.68	2.439
C12	-1.693	-0.004	4.744
H13	-2.765	-0.145	4.532
H14	-1.602	0.405	5.754
O15	-0.987	-1.233	4.738
H16	-1.105	-1.657	3.861
O17	-1.199	2.904	5.393
H18	-0.226	2.88	5.407
O19	-1.768	4.737	3.225
H20	-1.541	4.998	4.134
O21	-1.217	3.812	0.607
H22	-1.455	4.716	0.876
O23	0.256	1.556	1.298
C24	0.849	0.765	0.275
C25	2.292	0.341	0.702
C26	2.346	-1.162	0.311
C27	0.881	-1.596	0.476
H28	3.043	0.895	0.127
H29	3.02	-1.711	0.977
H30	0.623	-2.396	-0.224
C31	0.821	1.584	-1.021
H32	1.349	2.527	-0.85
H33	-0.219	1.815	-1.279
O34	1.427	0.827	-2.076
H35	1.946	1.428	-2.631
O36	2.46	0.556	2.094
H37	3.383	0.339	2.303

O38	2.822	-1.354	-1.008
H39	2.346	-0.707	-1.574
C40	0.499	-1.996	1.903
H41	0.931	-1.294	2.624
H42	0.896	-2.994	2.116
O43	-0.921	-2.072	2.063
H44	-1.255	-1.166	1.893
O45	0.127	-0.436	0.049

SCF GIAO Magnetic shielding tensor (ppm) of sucrose 235.out:

1 H Isotropic = 26.3850 Anisotropy = 2.4021

XX= 27.3039 YX= 0.1559 ZX= -1.4613

XY= 0.2128 YY= 25.0947 ZY= 1.5729

XZ= 0.1408 YZ= 1.3763 ZZ= 26.7563

Eigenvalues: 24.1544 27.0142 27.9864

2 C Isotropic = 89.6658 Anisotropy = 31.9192

XX= 82.0654 YX= 4.5239 ZX= -24.2139

XY= 6.2958 YY= 108.5797 ZY= -5.0976

XZ= -16.6784 YZ= 2.8586 ZZ= 78.3523

Eigenvalues: 59.5145 98.5377 110.9453

3 C Isotropic = 109.1868 Anisotropy = 29.2490

XX= 118.2596 YX= -7.8009 ZX= -1.7725

XY= -13.8979 YY= 116.7913 ZY= 4.1533

XZ= -0.9360 YZ= 2.3665 ZZ= 92.5097

Eigenvalues: 92.0793 106.7950 128.6862

4 C Isotropic = 104.7568 Anisotropy = 36.5936

XX= 105.2446 YX= 4.9622 ZX= 26.4754

XY= 0.4429 YY= 105.7476 ZY= 0.7033

XZ= 19.8534 YZ= 11.8630 ZZ= 103.2782

Eigenvalues: 80.7814 104.3364 129.1525

5 C Isotropic = 111.1961 Anisotropy = 37.5827

XX= 106.4545 YX= 5.0340 ZX= 22.3832

XY= -0.4979 YY= 110.4813 ZY= 3.8460

XZ= 20.4054 YZ= 13.7265 ZZ= 116.6526

Eigenvalues: 88.8899 108.4472 136.2513

6 C Isotropic = 112.7686 Anisotropy = 36.4716

XX= 107.4795 YX= 4.1867 ZX= 3.5938

XY= 14.0050 YY= 133.9931 ZY= -0.6564

XZ= -0.5849 YZ= -7.1552 ZZ= 96.8333

Eigenvalues: 95.8099 105.4130 137.0830

7 H Isotropic = 28.1877 Anisotropy = 7.0162

XX= 31.6522 YX= -2.3106 ZX= -1.0521

XY= -3.1752 YY= 26.5130 ZY= 0.0203

XZ= -0.0328 YZ= -0.5457 ZZ= 26.3977

Eigenvalues: 25.1537 26.5442 32.8651

8 H Isotropic = 27.8190 Anisotropy = 4.0906

XX= 29.3754 YX= 0.6931 ZX= 1.8734

XY= 1.4255 YY= 26.9291 ZY= 1.4802

XZ= 0.5811 YZ= 1.0319 ZZ= 27.1524

Eigenvalues: 25.7789 27.1320 30.5460

9 H Isotropic = 28.8141 Anisotropy = 1.5854

XX= 29.3564 YX= 0.0887 ZX= 0.1593

XY= 0.9467 YY= 27.7861 ZY= 0.1951

XZ= -1.0203 YZ= -0.4785 ZZ= 29.2997

Eigenvalues: 27.6307 28.9405 29.8710

10 H Isotropic = 28.1500 Anisotropy = 3.0149

XX= 26.5271 YX= 0.7571 ZX= -1.9417

XY= 0.9243 YY= 28.8943 ZY= -0.5850

XZ= -2.0717 YZ= 1.2007 ZZ= 29.0287

Eigenvalues: 25.2013 29.0888 30.1600

11 O Isotropic = 215.0434 Anisotropy = 71.6587

XX= 184.8376 YX= 20.7821 ZX= -33.1683

XY= 18.1826 YY= 240.9219 ZY= -27.5598

XZ= -16.1450 YZ= -9.3932 ZZ= 219.3708

Eigenvalues: 170.7208 211.5935 262.8159

12 C Isotropic = 122.1302 Anisotropy = 54.3084

XX= 130.5488 YX= -24.6479 ZX= -13.2418

XY= -19.6165 YY= 139.2656 ZY= 1.4750

XZ= -8.0467 YZ= -0.1903 ZZ= 96.5762

Eigenvalues: 92.6624 115.3923 158.3358

13 H Isotropic = 28.2102 Anisotropy = 5.5396

XX= 29.2433 YX= -0.5911 ZX= -4.5361

XY= -0.7680 YY= 28.7336 ZY= -0.6930

XZ= -2.9197 YZ= -1.7606 ZZ= 26.6537

Eigenvalues: 23.6220 29.1053 31.9033

14 H Isotropic = 28.0121 Anisotropy = 5.5422

XX= 30.8441 YX= 0.5269 ZX= 3.2559

XY= -0.9559 YY= 30.1613 ZY= -0.4740

XZ= 2.1449 YZ= 0.6607 ZZ= 23.0309

Eigenvalues: 22.1854 30.1440 31.7069

15 O Isotropic = 299.5103 Anisotropy = 17.5697

XX= 310.1991 YX= -11.3916 ZX= -0.8817

XY= 5.1706 YY= 301.4345 ZY= -0.4576

XZ= 2.7816 YZ= 0.5537 ZZ= 286.8973

Eigenvalues: 286.8564 300.4510 311.2234

16 H Isotropic = 26.5482 Anisotropy = 25.3096

XX= 36.2064 YX= 3.3556 ZX= 12.0787

XY= 2.3776 YY= 21.8740 ZY= 2.8892

XZ= 11.4509 YZ= 2.5338 ZZ= 21.5644

Eigenvalues: 14.8808 21.3426 43.4213

17 O Isotropic = 284.7215 Anisotropy = 80.6741

XX= 269.6053 YX= 6.5825 ZX= -36.3829

XY= 12.3316 YY= 252.8595 ZY= -1.8444

XZ= -6.9216 YZ= 8.0484 ZZ= 331.6995

Eigenvalues: 246.7057 268.9544 338.5042

18 H Isotropic = 31.1244 Anisotropy = 14.8253

XX= 29.4552 YX= 0.1982 ZX= -2.6431

XY= 0.8111 YY= 23.6472 ZY= 1.3331

XZ= -2.7775 YZ= 1.5551 ZZ= 40.2706

Eigenvalues: 23.4263 28.9390 41.0079

19 O Isotropic = 292.7639 Anisotropy = 46.1089

XX= 322.0552 YX= -19.3758 ZX= 6.4944

XY= 4.4916 YY= 267.3319 ZY= 1.3149

XZ= -11.4492 YZ= 19.8697 ZZ= 288.9046

Eigenvalues: 262.3985 292.3900 323.5032

20 H Isotropic = 29.2070 Anisotropy = 17.0911

XX= 32.7606 YX= -0.6086 ZX= 9.7516

XY= -1.5243 YY= 26.6769 ZY= 3.4759

XZ= 9.8314 YZ= 2.4196 ZZ= 28.1834

Eigenvalues: 19.2239 27.7960 40.6010

21 O Isotropic = 292.5878 Anisotropy = 38.1888

XX= 296.5319 YX= -11.8886 ZX= 4.3869

XY= -9.7513 YY= 310.9031 ZY= -6.4239

XZ= -6.3224 YZ= -12.5685 ZZ= 270.3284

Eigenvalues: 267.8042 291.9122 318.0470

22 H Isotropic = 29.4893 Anisotropy = 18.1797

XX= 33.3326 YX= -6.9182 ZX= 2.9417

XY= -6.7076 YY= 35.4527 ZY= -0.9333

XZ= 3.8600 YZ= -0.1782 ZZ= 19.6827

Eigenvalues: 18.8062 28.0527 41.6091

23 O Isotropic = 211.7530 Anisotropy = 38.0550

XX= 210.5131 YX= 4.6755 ZX= 4.5544

XY= 8.9382 YY= 214.2979 ZY= -29.9281

XZ= -15.9546 YZ= -13.4879 ZZ= 210.4480

Eigenvalues: 190.5713 207.5647 237.1230

24 C Isotropic = 72.5390 Anisotropy = 25.7893

XX= 81.0875 YX= -9.5614 ZX= 10.6534

XY= -7.7420 YY= 62.6286 ZY= -12.1869

XZ= -5.4156 YZ= -15.8788 ZZ= 73.9008

Eigenvalues: 51.9630 75.9221 89.7318

25 C Isotropic = 100.5031 Anisotropy = 25.4158

XX= 105.1986 YX= -5.0485 ZX= 18.0861

XY= -8.1031 YY= 96.4014 ZY= 3.2639

XZ= 10.5428 YZ= 4.5785 ZZ= 99.9094

Eigenvalues: 83.7965 100.2659 117.4470

26 C Isotropic = 103.9794 Anisotropy = 26.0769

XX= 117.7187 YX= -2.4653 ZX= 0.1261

XY= 8.0657 YY= 94.5876 ZY= -8.4347

XZ= 17.5631 YZ= 0.0251 ZZ= 99.6318

Eigenvalues: 90.2852 100.2889 121.3640

27 C Isotropic = 94.2420 Anisotropy = 43.3462

XX= 92.2441 YX= -13.4819 ZX= -19.6027

XY= -22.2472 YY= 103.4767 ZY= -1.4755

XZ= -19.9222 YZ= 8.2361 ZZ= 87.0053

Eigenvalues: 66.9230 92.6636 123.1395

28 H Isotropic = 27.4854 Anisotropy = 3.6020

XX= 26.7267 YX= 2.8803 ZX= 0.0196

XY= 3.1011 YY= 27.0509 ZY= -0.8026

XZ= 0.5665 YZ= 0.0878 ZZ= 28.6787

Eigenvalues: 23.8501 28.7194 29.8868

29 H Isotropic = 28.2340 Anisotropy = 4.8982

XX= 30.0059 YX= 0.1693 ZX= -1.6890

XY= -0.0943 YY= 27.3927 ZY= 2.9137

XZ= -2.2390 YZ= 2.3326 ZZ= 27.3033

Eigenvalues: 24.3431 28.8593 31.4995

30 H Isotropic = 27.5741 Anisotropy = 7.5165

XX= 29.3558 YX= -2.3844 ZX= 2.4410

XY= -2.8050 YY= 28.7110 ZY= -2.1038

XZ= 1.6371 YZ= -1.5147 ZZ= 24.6556

Eigenvalues: 23.7184 26.4188 32.5852

31 C Isotropic = 119.2945 Anisotropy = 50.6101

XX= 150.7166 YX= 8.9546 ZX= 5.2972

XY= 6.5388 YY= 108.7247 ZY= 6.1509

XZ= 6.8049 YZ= 6.8689 ZZ= 98.4422

Eigenvalues: 95.2026 109.6463 153.0345

32 H Isotropic = 28.1406 Anisotropy = 4.3002

XX= 30.5517 YX= -0.2376 ZX= 1.8233

XY= 0.0513 YY= 29.3357 ZY= -1.8307

XZ= 0.5371 YZ= -2.4394 ZZ= 24.5344

Eigenvalues: 23.5577 29.8567 31.0074

33 H Isotropic = 28.0868 Anisotropy = 6.2690

XX= 32.0095 YX= 0.4650 ZX= -1.9920

XY= 0.7599 YY= 27.1810 ZY= 3.3726

XZ= -0.7256 YZ= 2.8841 ZZ= 25.0699

Eigenvalues: 22.5968 29.3975 32.2662

34 O Isotropic = 305.6953 Anisotropy = 66.6961

XX= 309.7748 YX= 10.8647 ZX= 2.3240

XY= 28.3878 YY= 338.7422 ZY= -11.0477

XZ= -1.2237 YZ= -14.2504 ZZ= 268.5690

Eigenvalues: 265.9632 300.9634 350.1594

35 H Isotropic = 30.0090 Anisotropy = 20.7824

XX= 30.0246 YX= 7.9676 ZX= -1.7086

XY= 7.6033 YY= 37.7419 ZY= -5.2234

XZ= -2.1450 YZ= -4.8019 ZZ= 22.2604

Eigenvalues: 20.7569 25.4062 43.8639

36 O Isotropic = 278.0662 Anisotropy = 68.0186

XX= 270.7448 YX= -26.8629 ZX= -25.5737

XY= -10.3523 YY= 266.7869 ZY= 30.9324

XZ= -8.3255 YZ= 22.3777 ZZ= 296.6669

Eigenvalues: 247.3154 263.4713 323.4120

37 H Isotropic = 30.3148 Anisotropy = 19.0642

XX= 27.9207 YX= -0.0281 ZX= -4.1519

XY= -1.1076 YY= 23.1226 ZY= 6.3341

XZ= -4.3882 YZ= 5.6884 ZZ= 39.9010

Eigenvalues: 21.0930 26.8272 43.0243

38 O Isotropic = 275.2851 Anisotropy = 25.0081

XX= 279.0526 YX= 3.6604 ZX= 6.6752

XY= 8.3605 YY= 274.1721 ZY= -10.7580

XZ= 23.6123 YZ= -13.0033 ZZ= 272.6307

Eigenvalues: 252.4792 281.4191 291.9572

39 H Isotropic = 26.6862 Anisotropy = 20.8491

XX= 25.7177 YX= -3.2367 ZX= -1.8030

XY= -2.6360 YY= 35.1349 ZY= 9.9659

XZ= -1.4579 YZ= 9.7140 ZZ= 19.2060

Eigenvalues: 14.5072 24.9657 40.5856

40 C Isotropic = 124.6627 Anisotropy = 53.6457

XX= 125.5732 YX= 14.9421 ZX= -29.7718

XY= 9.9738 YY= 112.9518 ZY= 0.4239

XZ= -24.7921 YZ= -5.8386 ZZ= 135.4630

Eigenvalues: 98.1287 115.4328 160.4265

41 H Isotropic = 27.6724 Anisotropy = 5.3789

XX= 27.1406 YX= 2.7339 ZX= -2.3131

XY= 2.1387 YY= 26.7192 ZY= -1.5357

XZ= 0.1049 YZ= -1.8869 ZZ= 29.1575

Eigenvalues: 24.4175 27.3414 31.2584

42 H Isotropic = 28.4902 Anisotropy = 6.7450

XX= 28.3059 YX= -2.3678 ZX= -2.7141

XY= -1.7487 YY= 31.2753 ZY= 0.2910

XZ= -2.9298 YZ= 1.3995 ZZ= 25.8893

Eigenvalues: 23.9997 28.4840 32.9868

43 O Isotropic = 292.2680 Anisotropy = 26.7141

XX= 285.7467 YX= -2.6513 ZX= 5.8052

XY= -10.9151 YY= 307.6352 ZY= 6.2218

XZ= -8.1667 YZ= 0.7773 ZZ= 283.4221

Eigenvalues: 282.8786 283.8479 310.0774

44 H Isotropic = 27.3110 Anisotropy = 21.3333

XX= 30.2793 YX= -8.9853 ZX= -2.8304

XY= -10.3294 YY= 33.1782 ZY= -1.0016

XZ= -1.8133 YZ= -0.5138 ZZ= 18.4753

Eigenvalues: 17.3399 23.0598 41.5331

45 O Isotropic = 222.6469 Anisotropy = 119.7012

XX= 193.7888 YX= -45.8710 ZX= -21.0221

XY= -45.2319 YY= 222.2846 ZY= -57.2605

XZ= 3.6476 YZ= -60.4115 ZZ= 251.8673

Eigenvalues: 141.7669 223.7261 302.4477

Energy for the sucrose conformer 355: -1297.58

The coordinates of the sucrose 355.out:

H1	-1.593	1.165	0.476
C2	-1.148	1.572	1.383
C3	-1.194	3.49	3.002
C4	-1.234	1.108	3.777
C5	-1.717	2.535	4.075
C6	-1.615	3.015	1.614
H7	-0.101	3.523	3.057
H8	-0.142	1.078	3.869
H9	-2.821	2.546	4.054
H10	-2.717	2.99	1.573
O11	-1.62	0.735	2.428
C12	-1.834	0.075	4.731
H13	-2.897	-0.061	4.474
H14	-1.784	0.49	5.742
O15	-1.133	-1.155	4.763
H16	-1.224	-1.591	3.889
O17	-1.239	2.907	5.359
H18	-1.355	3.871	5.419
O19	-1.607	4.839	3.243
H20	-2.58	4.871	3.209
O21	-1.099	3.843	0.59
H22	-1.221	4.758	0.899
O23	0.267	1.532	1.293
C24	0.841	0.751	0.238
C25	2.285	0.341	0.688
C26	2.323	-1.174	0.38
C27	0.864	-1.596	0.542
H28	3.034	0.878	0.093
H29	3.007	-1.693	1.06
H30	0.616	-2.428	-0.122
C31	0.799	1.553	-1.069
H32	1.156	2.567	-0.868
H33	-0.25	1.623	-1.394
O34	1.618	0.995	-2.082
H35	1.655	0.026	-1.957

O36	2.51	0.542	2.07
H37	1.869	1.218	2.357
O38	2.661	-1.428	-0.987
H39	3.578	-1.138	-1.132
C40	0.455	-1.933	1.977
H41	0.857	-1.194	2.678
H42	0.865	-2.912	2.245
O43	-0.966	-2.031	2.098
H44	-1.313	-1.136	1.901
O45	0.126	-0.457	0.036

SCF GIAO Magnetic shielding tensor (ppm) of sucrose 355.out:

1 H Isotropic = 26.3074 Anisotropy = 2.2816

XX= 27.4502 YX= 0.4154 ZX= -1.3109

XY= 0.4029 YY= 24.7994 ZY= 1.5324

XZ= 0.1337 YZ= 1.3165 ZZ= 26.6727

Eigenvalues: 23.9146 27.1792 27.8285

2 C Isotropic = 88.7366 Anisotropy = 32.1182

XX= 82.7812 YX= 4.7450 ZX= -23.8833

XY= 6.4553 YY= 107.4531 ZY= -4.8003

XZ= -17.4684 YZ= 2.5377 ZZ= 75.9756

Eigenvalues: 58.2675 97.7937 110.1488

3 C Isotropic = 108.2032 Anisotropy = 32.6198

XX= 118.0103 YX= -8.7157 ZX= 1.5381

XY= -14.3674 YY= 118.2521 ZY= 5.7655

XZ= 1.6731 YZ= 6.7997 ZZ= 88.3471

Eigenvalues: 86.5464 108.1134 129.9497

4 C Isotropic = 104.0567 Anisotropy = 36.1034

XX= 105.1818 YX= 4.9647 ZX= 25.1476

XY= 1.1088 YY= 105.7117 ZY= 1.1482

XZ= 20.9414 YZ= 10.8092 ZZ= 101.2767

Eigenvalues: 79.8815 104.1630 128.1256

5 C Isotropic = 112.8592 Anisotropy = 36.4474

XX= 112.1623 YX= 8.1108 ZX= 19.9150

XY= 1.5094 YY= 106.8507 ZY= 4.0340

XZ= 16.1808 YZ= 12.1729 ZZ= 119.5645

Eigenvalues: 97.1747 104.2454 137.1574

6 C Isotropic = 112.8453 Anisotropy = 34.2680

XX= 109.2470 YX= 4.4301 ZX= 1.9286

XY= 15.0865 YY= 131.8012 ZY= -0.0446

XZ= -2.4150 YZ= -6.4147 ZZ= 97.4879

Eigenvalues: 97.1396 105.7058 135.6907

7 H Isotropic = 28.2987 Anisotropy = 6.7374

XX= 31.6111 YX= -2.4746 ZX= -0.8391

XY= -2.8659 YY= 26.6533 ZY= 0.3275

XZ= 0.1532 YZ= -0.4022 ZZ= 26.6316

Eigenvalues: 25.4633 26.6425 32.7903

8 H Isotropic = 27.8902 Anisotropy = 4.1157

XX= 29.3590 YX= 0.6619 ZX= 2.0508

XY= 1.3947 YY= 27.0405 ZY= 1.4261

XZ= 0.6652 YZ= 0.9868 ZZ= 27.2712

Eigenvalues: 25.9336 27.1031 30.6340

9 H Isotropic = 28.6874 Anisotropy = 1.9187

XX= 29.1569 YX= 0.1989 ZX= 0.1720

XY= 1.2351 YY= 27.3404 ZY= 0.4642

XZ= -1.1633 YZ= -0.4707 ZZ= 29.5648

Eigenvalues: 27.0809 29.0148 29.9665

10 H Isotropic = 28.3460 Anisotropy = 3.1383

XX= 26.8123 YX= 0.8514 ZX= -1.9926

XY= 0.9079 YY= 28.9385 ZY= -0.5720

XZ= -2.0425 YZ= 1.1686 ZZ= 29.2872

Eigenvalues: 25.4439 29.1559 30.4382

11 O Isotropic = 219.3243 Anisotropy = 72.3331

XX= 190.1398 YX= 18.7317 ZX= -35.4799

XY= 18.1368 YY= 245.7609 ZY= -27.8883

XZ= -18.0534 YZ= -9.5637 ZZ= 222.0721

Eigenvalues: 174.1894 216.2371 267.5463

12 C Isotropic = 122.2192 Anisotropy = 53.5103

XX= 129.3602 YX= -24.0598 ZX= -13.8075

XY= -19.0190 YY= 139.8601 ZY= 2.4906

XZ= -8.8176 YZ= 0.3495 ZZ= 97.4374

Eigenvalues: 93.0841 115.6809 157.8928

13 H Isotropic = 28.2423 Anisotropy = 5.5724

XX= 29.1319 YX= -0.5440 ZX= -4.5692

XY= -0.7221 YY= 28.7550 ZY= -0.6233

XZ= -3.0124 YZ= -1.6923 ZZ= 26.8402

Eigenvalues: 23.6884 29.0813 31.9573

14 H Isotropic = 27.9925 Anisotropy = 5.5696

XX= 30.9443 YX= 0.5424 ZX= 3.1123

XY= -0.8405 YY= 30.1795 ZY= -0.3775

XZ= 2.0579 YZ= 0.7300 ZZ= 22.8536

Eigenvalues: 22.0927 30.1793 31.7055

15 O Isotropic = 298.7980 Anisotropy = 17.6949

XX= 309.5466 YX= -11.4831 ZX= -1.5668

XY= 5.0085 YY= 300.5794 ZY= -0.8685

XZ= 2.0548 YZ= 1.1542 ZZ= 286.2680

Eigenvalues: 286.2632 299.5362 310.5946

16 H Isotropic = 26.6521 Anisotropy = 25.1312

XX= 36.7714 YX= 2.9851 ZX= 11.7776

XY= 2.0486 YY= 21.9103 ZY= 2.6705

XZ= 11.1885 YZ= 2.2367 ZZ= 21.2745

Eigenvalues: 15.0205 21.5296 43.4062

17 O Isotropic = 291.1344 Anisotropy = 42.8906

XX= 282.3932 YX= -16.6239 ZX= 7.4442

XY= -18.8637 YY= 287.7006 ZY= -14.6040

XZ= 26.2242 YZ= 1.7402 ZZ= 303.3094

Eigenvalues: 264.8119 288.8632 319.7281

18 H Isotropic = 29.3229 Anisotropy = 17.2953

XX= 32.3112 YX= -6.5225 ZX= 7.5534

XY= -6.8809 YY= 31.9235 ZY= -0.0345

XZ= 6.9464 YZ= -1.2796 ZZ= 23.7338

Eigenvalues: 18.9035 28.2121 40.8531

19 O Isotropic = 290.6872 Anisotropy = 118.1844

XX= 302.6867 YX= -27.7223 ZX= -44.5181

XY= -9.8045 YY= 253.3166 ZY= -15.8238

XZ= -72.9943 YZ= 10.5109 ZZ= 316.0582

Eigenvalues: 235.5545 267.0303 369.4768

20 H Isotropic = 31.3405 Anisotropy = 17.3410

XX= 34.3496 YX= -3.6220 ZX= -8.1976

XY= -3.4964 YY= 26.0622 ZY= 0.7297

XZ= -8.3734 YZ= 1.1843 ZZ= 33.6098

Eigenvalues: 23.8198 27.3005 42.9012

21 O Isotropic = 293.1419 Anisotropy = 36.5865

XX= 297.5935 YX= -7.6444 ZX= 7.6479

XY= -10.3565 YY= 308.4431 ZY= -9.7597

XZ= -5.3040 YZ= -18.9525 ZZ= 273.3889

Eigenvalues: 268.1264 293.7663 317.5329

22 H Isotropic = 29.3268 Anisotropy = 17.8612

XX= 32.7691 YX= -6.4789 ZX= 4.2638

XY= -6.0984 YY= 34.8993 ZY= -2.3579

XZ= 5.3484 YZ= -1.5033 ZZ= 20.3121

Eigenvalues: 18.6704 28.0758 41.2343

23 O Isotropic = 208.1599 Anisotropy = 41.3138

XX= 208.2323 YX= 7.5533 ZX= 5.1693

XY= 10.4984 YY= 215.6597 ZY= -29.5657

XZ= -19.3505 YZ= -13.4573 ZZ= 200.5877

Eigenvalues: 185.3146 203.4626 235.7025

24 C Isotropic = 71.1014 Anisotropy = 27.5664

XX= 77.0424 YX= -10.1718 ZX= 9.1309

XY= -9.5983 YY= 66.8354 ZY= -13.3666

XZ= -4.5229 YZ= -17.0413 ZZ= 69.4266

Eigenvalues: 51.4709 72.3544 89.4791

25 C Isotropic = 104.5490 Anisotropy = 29.6762

XX= 107.4976 YX= -2.4053 ZX= 20.8842

XY= -7.0066 YY= 97.3800 ZY= 0.9383

XZ= 11.1966 YZ= 2.6613 ZZ= 108.7693

Eigenvalues: 89.3588 99.9550 124.3331

26 C Isotropic = 104.7254 Anisotropy = 28.3358

XX= 121.1487 YX= -2.0858 ZX= -0.2260

XY= 7.3031 YY= 99.2290 ZY= -6.4828

XZ= 17.0136 YZ= -0.8203 ZZ= 93.7986

Eigenvalues: 89.5687 100.9915 123.6160

27 C Isotropic = 95.6567 Anisotropy = 46.7871

XX= 91.2495 YX= -13.2522 ZX= -20.9925

XY= -21.0128 YY= 108.3378 ZY= 1.4380

XZ= -20.9891 YZ= 11.7074 ZZ= 87.3829

Eigenvalues: 66.9459 93.1762 126.8481

28 H Isotropic = 27.4528 Anisotropy = 4.4547

XX= 26.7466 YX= 2.9375 ZX= -0.3243

XY= 3.7336 YY= 27.2447 ZY= -1.0896

XZ= 0.6631 YZ= -0.3307 ZZ= 28.3669

Eigenvalues: 23.5735 28.3622 30.4226

29 H Isotropic = 27.6446 Anisotropy = 4.8985

XX= 29.4387 YX= 0.2870 ZX= -1.3910

XY= -0.6343 YY= 26.7896 ZY= 3.5622

XZ= -1.7049 YZ= 2.5729 ZZ= 26.7055

Eigenvalues: 23.5110 28.5125 30.9103

30 H Isotropic = 27.4940 Anisotropy = 7.4512

XX= 29.2010 YX= -2.4061 ZX= 2.2605

XY= -2.8427 YY= 28.7853 ZY= -2.1515

XZ= 1.2764 YZ= -1.6220 ZZ= 24.4958

Eigenvalues: 23.6491 26.3715 32.4615

31 C Isotropic = 119.6324 Anisotropy = 47.9876

XX= 149.2881 YX= 13.1090 ZX= -0.3521

XY= 5.7277 YY= 109.8281 ZY= 3.1589

XZ= 5.6662 YZ= 2.7415 ZZ= 99.7810

Eigenvalues: 98.9786 108.2945 151.6241

32 H Isotropic = 28.3514 Anisotropy = 4.9476

XX= 31.4118 YX= -0.7560 ZX= 1.0219

XY= -0.0820 YY= 29.7906 ZY= -1.2835

XZ= 0.0845 YZ= -2.1736 ZZ= 23.8518

Eigenvalues: 23.3628 30.0416 31.6498

33 H Isotropic = 28.1021 Anisotropy = 5.3856

XX= 31.1117 YX= 0.8897 ZX= -2.2904

XY= 1.3671 YY= 26.8180 ZY= 3.2345

XZ= -1.2106 YZ= 2.9165 ZZ= 26.3767

Eigenvalues: 22.9948 29.6191 31.6925

34 O Isotropic = 308.4663 Anisotropy = 72.7254

XX= 309.2784 YX= -17.4110 ZX= 4.0813

XY= -34.6974 YY= 342.5789 ZY= -3.1931

XZ= 0.6626 YZ= -0.8323 ZZ= 273.5416

Eigenvalues: 273.3832 295.0658 356.9499

35 H Isotropic = 28.7914 Anisotropy = 19.0430

XX= 30.3302 YX= -6.4708 ZX= 1.4803

XY= -6.7567 YY= 37.5636 ZY= 1.0442

XZ= 2.0100 YZ= 1.4843 ZZ= 18.4803

Eigenvalues: 17.9352 26.9522 41.4867

36 O Isotropic = 292.7156 Anisotropy = 55.8171

XX= 314.7521 YX= -24.1104 ZX= -0.9645

XY= -26.0251 YY= 283.8702 ZY= 11.6015

XZ= -6.4846 YZ= 6.4229 ZZ= 279.5246

Eigenvalues: 266.7688 281.4511 329.9270

37 H Isotropic = 28.5980 Anisotropy = 18.0020

XX= 38.3892 YX= -4.5822 ZX= -3.0095

XY= -5.3481 YY= 20.1832 ZY= 3.4691

XZ= -2.2232 YZ= 4.2919 ZZ= 27.2216

Eigenvalues: 17.8207 27.3740 40.5994

38 O Isotropic = 273.4789 Anisotropy = 72.1003

XX= 277.6495 YX= 15.2193 ZX= -3.3207

XY= 26.9973 YY= 259.6641 ZY= -36.8437

XZ= -15.4520 YZ= -40.9354 ZZ= 283.1230

Eigenvalues: 227.9079 270.9830 321.5458

39 H Isotropic = 30.1679 Anisotropy = 18.2354

XX= 33.5067 YX= 5.1634 ZX= -6.7428

XY= 5.8140 YY= 25.2944 ZY= -5.1692

XZ= -6.4459 YZ= -4.2259 ZZ= 31.7027

Eigenvalues: 22.2289 25.9500 42.3249

40 C Isotropic = 124.7761 Anisotropy = 52.8217

XX= 124.9709 YX= 15.7139 ZX= -28.3022

XY= 10.6645 YY= 113.0629 ZY= -0.7444

XZ= -23.6217 YZ= -7.0263 ZZ= 136.2947

Eigenvalues: 98.9235 115.4143 159.9906

41 H Isotropic = 27.7144 Anisotropy = 5.4641

XX= 27.1811 YX= 2.7532 ZX= -2.1441

XY= 2.2033 YY= 27.0615 ZY= -1.7952

XZ= 0.3931 YZ= -2.2336 ZZ= 28.9005

Eigenvalues: 24.4533 27.3327 31.3571

42 H Isotropic = 28.4486 Anisotropy = 6.8274

XX= 28.0006 YX= -2.0749 ZX= -2.8983

XY= -1.4626 YY= 31.3593 ZY= 0.7116

XZ= -2.9637 YZ= 1.8517 ZZ= 25.9857

Eigenvalues: 23.8938 28.4517 33.0002

43 O Isotropic = 292.4861 Anisotropy = 24.8505

XX= 286.8507 YX= -2.9580 ZX= 6.0853

XY= -10.4215 YY= 306.3012 ZY= 6.4299

XZ= -7.6425 YZ= 1.6333 ZZ= 284.3065

Eigenvalues: 283.4791 284.9262 309.0531

44 H Isotropic = 27.5068 Anisotropy = 20.7422

XX= 30.1721 YX= -8.6773 ZX= -3.3421

XY= -10.0279 YY= 33.2575 ZY= -0.3399

XZ= -2.3816 YZ= 0.1035 ZZ= 19.0909

Eigenvalues: 17.8066 23.3790 41.3350

45 O Isotropic = 218.0173 Anisotropy = 125.0548

XX= 179.1473 YX= -42.6079 ZX= -19.5472

XY= -46.6457 YY= 233.3190 ZY= -55.8915

XZ= 1.0833 YZ= -61.4871 ZZ= 241.5856

Eigenvalues: 138.1414 214.5234 301.3872

Energy for the sucrose conformer 1: -1297.6

The coordinates of the sucrose 1.out:

H1	-1.704	0.956	0.44
C2	-1.201	1.391	1.306
C3	-1.116	3.38	2.852
C4	-1.069	1.041	3.693
C5	-1.573	2.46	3.982
C6	-1.601	2.862	1.495
H7	-0.015	3.4	2.854
H8	0.025	1.063	3.622
H9	-2.674	2.456	4.016
H10	-2.696	2.912	1.484
O11	-1.623	0.615	2.418
C12	-1.45	0.004	4.747
H13	-2.499	-0.293	4.593
H14	-1.375	0.477	5.729
O15	-0.576	-1.114	4.772
H16	-0.635	-1.576	3.91
O17	-1.036	2.886	5.229
H18	-1.197	3.844	5.275
O19	-1.628	4.681	3.12
H20	-1.383	5.231	2.356
O21	-1.156	3.688	0.432
H22	-0.216	3.477	0.231
O23	0.205	1.305	1.173
C24	0.742	0.629	0.029
C25	2.16	0.189	0.416
C26	1.887	-1.101	1.192
C27	0.763	-1.713	0.331
H28	2.694	-0.089	-0.505
H29	1.522	-0.862	2.197
H30	1.228	-2.275	-0.49
C31	0.688	1.564	-1.183
H32	-0.348	1.728	-1.492
H33	1.229	1.105	-2.02
O34	1.228	2.843	-0.85

H35	2.029	2.69	-0.311
O36	2.844	1.228	1.092
H37	3.777	0.965	1.162
O38	3.063	-1.892	1.241
H39	2.984	-2.511	1.983
C40	-0.245	-2.625	1.015
H41	0.273	-3.527	1.358
H42	-0.994	-2.933	0.272
O43	-0.88	-2.058	2.153
H44	-1.253	-1.181	1.929
O45	0.06	-0.571	-0.251

SCF GIAO Magnetic shielding tensor (ppm) of sucrose 1.out:

1 H Isotropic = 26.4826 Anisotropy = 2.3972

XX= 26.6256 YX= 0.4414 ZX= -1.3480

XY= 0.5406 YY= 25.2323 ZY= 0.8214

XZ= -0.2460 YZ= 0.4798 ZZ= 27.5899

Eigenvalues: 24.7953 26.5718 28.0807

2 C Isotropic = 90.6756 Anisotropy = 37.4537

XX= 83.1113 YX= -2.1089 ZX= -20.8701

XY= 1.4832 YY= 115.3686 ZY= -8.8879

XZ= -16.6997 YZ= 2.6840 ZZ= 73.5468

Eigenvalues: 58.8215 97.5606 115.6447

3 C Isotropic = 107.9114 Anisotropy = 27.3439

XX= 119.7753 YX= -6.1526 ZX= -2.2848

XY= -13.1369 YY= 109.2185 ZY= 4.8824

XZ= -1.1616 YZ= 6.7971 ZZ= 94.7405

Eigenvalues: 92.5654 105.0282 126.1407

4 C Isotropic = 104.6795 Anisotropy = 34.6060

XX= 100.6809 YX= 1.4095 ZX= 23.0024

XY= -1.6191 YY= 106.3044 ZY= 8.2546

XZ= 16.5436 YZ= 15.0599 ZZ= 107.0531

Eigenvalues: 81.3199 104.9684 127.7502

5 C Isotropic = 113.7314 Anisotropy = 41.4799

XX= 110.3528 YX= 7.2547 ZX= 21.2224

XY= 0.8635 YY= 106.4286 ZY= 7.6978

XZ= 16.3032 YZ= 15.2304 ZZ= 124.4128

Eigenvalues: 95.9253 103.8842 141.3847

6 C Isotropic = 111.8326 Anisotropy = 33.5815

XX= 106.0842 YX= 1.2234 ZX= 6.9642

XY= 9.6235 YY= 133.1379 ZY= 2.1215

XZ= 3.7476 YZ= -6.5225 ZZ= 96.2758

Eigenvalues: 93.4608 107.8168 134.2203

7 H Isotropic = 28.1679 Anisotropy = 6.8886

XX= 32.5983 YX= -0.9445 ZX= -0.8273

XY= -1.1874 YY= 25.5753 ZY= 0.1106

XZ= 0.4340 YZ= -0.6535 ZZ= 26.3299

Eigenvalues: 25.3285 26.4148 32.7602

8 H Isotropic = 27.7111 Anisotropy = 3.4981

XX= 28.2988 YX= 0.5742 ZX= 1.7286

XY= 1.2330 YY= 27.9587 ZY= 1.9258

XZ= 0.3941 YZ= 1.0122 ZZ= 26.8757

Eigenvalues: 25.7871 27.3030 30.0431

9 H Isotropic = 28.4847 Anisotropy = 2.1778

XX= 28.6706 YX= 0.8482 ZX= 0.2231

XY= 1.8797 YY= 27.3140 ZY= 0.3309

XZ= -0.9986 YZ= -0.7626 ZZ= 29.4695

Eigenvalues: 26.4688 29.0487 29.9365

10 H Isotropic = 28.4489 Anisotropy = 3.4268

XX= 27.0537 YX= 0.5270 ZX= -1.8212

XY= 0.7042 YY= 28.8903 ZY= -0.7343

XZ= -2.4696 YZ= 0.7068 ZZ= 29.4028

Eigenvalues: 25.6963 28.9170 30.7335

11 O Isotropic = 216.8768 Anisotropy = 72.0806

XX= 186.1560 YX= 6.2077 ZX= -24.9369

XY= 3.6262 YY= 256.1885 ZY= -29.7173

XZ= -15.6815 YZ= -9.3953 ZZ= 208.2858

Eigenvalues: 173.6481 212.0517 264.9305

12 C Isotropic = 123.1348 Anisotropy = 52.4009

XX= 141.5142 YX= -20.4494 ZX= -19.3923

XY= -16.0492 YY= 126.2730 ZY= 3.6364

XZ= -13.1381 YZ= 3.9826 ZZ= 101.6171

Eigenvalues: 95.5608 115.7748 158.0687

13 H Isotropic = 28.2734 Anisotropy = 5.5580

XX= 29.0632 YX= 0.5863 ZX= -4.0823

XY= 0.0734 YY= 29.0052 ZY= -1.5153

XZ= -2.3787 YZ= -2.1524 ZZ= 26.7518

Eigenvalues: 24.1081 28.7334 31.9788

14 H Isotropic = 27.9867 Anisotropy = 5.6380

XX= 31.1638 YX= 0.3906 ZX= 2.9566

XY= -0.7653 YY= 29.5455 ZY= 1.4252

XZ= 1.3423 YZ= 2.1293 ZZ= 23.2507

Eigenvalues: 22.2739 29.9407 31.7453

15 O Isotropic = 294.8488 Anisotropy = 19.3408

XX= 304.4666 YX= -2.9547 ZX= -4.8109

XY= 14.2755 YY= 297.6928 ZY= 0.6785

XZ= 1.4291 YZ= 0.0211 ZZ= 282.3872

Eigenvalues: 282.2154 294.5884 307.7427

16 H Isotropic = 27.0763 Anisotropy = 25.5190

XX= 34.7731 YX= 4.8261 ZX= 11.4848

XY= 3.9006 YY= 22.5984 ZY= 7.2391

XZ= 10.5717 YZ= 6.0570 ZZ= 23.8575

Eigenvalues: 15.0189 22.1211 44.0890

17 O Isotropic = 291.7951 Anisotropy = 42.2951

XX= 293.2508 YX= -13.3421 ZX= 11.8778

XY= -20.7609 YY= 280.4703 ZY= -12.7926

XZ= 22.2700 YZ= 5.3955 ZZ= 301.6643

Eigenvalues: 267.0410 288.3526 319.9919

18 H Isotropic = 29.4004 Anisotropy = 17.4331

XX= 35.7263 YX= -6.2135 ZX= 6.8276

XY= -6.5391 YY= 28.4893 ZY= 2.2935

XZ= 6.6537 YZ= 1.1187 ZZ= 23.9857

Eigenvalues: 18.8163 28.3624 41.0225

19 O Isotropic = 295.3140 Anisotropy = 43.8845

XX= 300.0894 YX= -13.0023 ZX= -8.5755

XY= -8.7224 YY= 312.1710 ZY= -2.2144

XZ= -39.1834 YZ= 9.9487 ZZ= 273.6816

Eigenvalues: 259.5037 301.8680 324.5703

20 H Isotropic = 29.2877 Anisotropy = 16.7891

XX= 28.0620 YX= -1.8717 ZX= 1.5465

XY= -1.8461 YY= 40.2022 ZY= 0.2250

XZ= 2.9134 YZ= 0.3683 ZZ= 19.5990

Eigenvalues: 19.0216 28.3612 40.4805

21 O Isotropic = 294.1353 Anisotropy = 59.7087

XX= 294.6193 YX= 35.1421 ZX= -26.1535

XY= 9.2233 YY= 301.1868 ZY= -0.1136

XZ= -34.8565 YZ= -9.2505 ZZ= 286.5997

Eigenvalues: 256.6385 291.8263 333.9411

22 H Isotropic = 27.0724 Anisotropy = 24.5745

XX= 35.2133 YX= 5.2157 ZX= -10.4926

XY= 5.0519 YY= 24.6210 ZY= -4.1333

XZ= -11.1126 YZ= -4.6577 ZZ= 21.3828

Eigenvalues: 15.2205 22.5412 43.4554

23 O Isotropic = 212.5841 Anisotropy = 41.8737

XX= 210.1754 YX= 1.7160 ZX= 9.2882

XY= 28.5742 YY= 222.2438 ZY= -14.0615

XZ= -26.1789 YZ= -14.9652 ZZ= 205.3332

Eigenvalues: 196.9799 200.2726 240.4999

24 C Isotropic = 79.3400 Anisotropy = 20.9040

XX= 86.9922 YX= 3.1434 ZX= 9.1693

XY= 3.2707 YY= 77.8601 ZY= -12.2714

XZ= 12.4062 YZ= -8.0966 ZZ= 73.1678

Eigenvalues: 60.7903 83.9538 93.2760

25 C Isotropic = 102.2993 Anisotropy = 28.6518

XX= 86.9236 YX= -14.2311 ZX= 0.9847

XY= -15.4208 YY= 103.0926 ZY= -6.1202

XZ= 12.3906 YZ= -0.5281 ZZ= 116.8817

Eigenvalues: 77.6893 107.8081 121.4005

26 C Isotropic = 110.5002 Anisotropy = 43.3217

XX= 113.9160 YX= -21.3089 ZX= -11.2163

XY= -26.3518 YY= 103.0945 ZY= 1.6362

XZ= -21.1786 YZ= -3.3820 ZZ= 114.4901

Eigenvalues: 80.3553 111.7640 139.3814

27 C Isotropic = 98.2906 Anisotropy = 51.3633

XX= 92.2981 YX= -30.4273 ZX= -15.6121

XY= -15.9600 YY= 100.6109 ZY= 10.7448

XZ= -16.2744 YZ= 13.2966 ZZ= 101.9628

Eigenvalues: 71.9703 90.3687 132.5328

28 H Isotropic = 27.5376 Anisotropy = 2.5735

XX= 28.5515 YX= 1.1382 ZX= -0.1021

XY= 1.0179 YY= 27.3381 ZY= -1.3774

XZ= 1.7928 YZ= 0.0312 ZZ= 26.7231

Eigenvalues: 25.6858 27.6737 29.2532

29 H Isotropic = 27.1497 Anisotropy = 6.6763

XX= 29.7729 YX= 1.2534 ZX= -2.5575

XY= 0.2474 YY= 26.0146 ZY= 0.7176

XZ= -3.9410 YZ= 0.0976 ZZ= 25.6616

Eigenvalues: 23.6511 26.1974 31.6006

30 H Isotropic = 27.9097 Anisotropy = 5.5924

XX= 31.4771 YX= -0.1485 ZX= 0.1426

XY= -1.4512 YY= 26.9670 ZY= 0.1762

XZ= 0.6549 YZ= -0.0699 ZZ= 25.2850

Eigenvalues: 25.2527 26.8384 31.6379

31 C Isotropic = 118.1575 Anisotropy = 46.0519

XX= 114.4687 YX= -15.6400 ZX= 19.1702

XY= -12.0765 YY= 128.5053 ZY= -14.0647

XZ= 15.1430 YZ= -13.3566 ZZ= 111.4985

Eigenvalues: 95.7379 109.8758 148.8588

32 H Isotropic = 28.2117 Anisotropy = 3.6986

XX= 26.6944 YX= -0.6717 ZX= 1.6353

XY= 0.2116 YY= 28.0474 ZY= 1.0062

XZ= 0.4092 YZ= 1.4487 ZZ= 29.8934

Eigenvalues: 26.1893 27.7684 30.6774

33 H Isotropic = 28.0789 Anisotropy = 6.0994

XX= 29.8308 YX= 2.3047 ZX= 2.3985

XY= 1.1635 YY= 28.9795 ZY= 0.0194

XZ= 2.9906 YZ= 1.1137 ZZ= 25.4264

Eigenvalues: 24.1364 27.9551 32.1452

34 O Isotropic = 294.8681 Anisotropy = 39.9087

XX= 274.0792 YX= 4.4952 ZX= -16.6328

XY= -6.0031 YY= 295.5593 ZY= 17.3129

XZ= 0.6851 YZ= 5.5702 ZZ= 314.9658

Eigenvalues: 272.4853 290.6451 321.4739

35 H Isotropic = 28.7080 Anisotropy = 15.8556

XX= 21.6489 YX= -4.0257 ZX= -3.5618

XY= -4.0523 YY= 27.0134 ZY= 2.6979

XZ= -3.6475 YZ= 2.6482 ZZ= 37.4618

Eigenvalues: 19.2614 27.5843 39.2784

36 O Isotropic = 293.0111 Anisotropy = 41.9171

XX= 293.7094 YX= -5.8181 ZX= -15.5453

XY= 2.7145 YY= 268.4272 ZY= 3.1736

XZ= -5.4837 YZ= -4.9392 ZZ= 316.8968

Eigenvalues: 268.2800 289.7975 320.9558

37 H Isotropic = 29.4587 Anisotropy = 19.7810

XX= 28.3953 YX= -0.5400 ZX= -7.8719

XY= -1.7103 YY= 21.8489 ZY= -3.1604

XZ= -7.7453 YZ= -2.4892 ZZ= 38.1320

Eigenvalues: 20.2341 25.4960 42.6461

38 O Isotropic = 297.2207 Anisotropy = 38.0170

XX= 307.3413 YX= 3.8767 ZX= -22.3368

XY= -5.7044 YY= 315.8594 ZY= 13.9024

XZ= -5.9283 YZ= 17.4219 ZZ= 268.4614

Eigenvalues: 260.0012 309.0956 322.5654

39 H Isotropic = 29.8814 Anisotropy = 18.8761

XX= 25.4490 YX= -2.9943 ZX= -4.4503

XY= -3.3026 YY= 39.5984 ZY= 5.5900

XZ= -4.6476 YZ= 5.0624 ZZ= 24.5967

Eigenvalues: 20.2423 26.9364 42.4654

40 C Isotropic = 124.3040 Anisotropy = 55.2553

XX= 150.4138 YX= 23.3555 ZX= 10.8352

XY= 18.7569 YY= 116.9631 ZY= -4.8391

XZ= 6.1533 YZ= -4.9172 ZZ= 105.5350

Eigenvalues: 97.7899 113.9811 161.1409

41 H Isotropic = 28.2519 Anisotropy = 7.8452

XX= 31.9222 YX= -3.6058 ZX= 0.0617

XY= -1.7952 YY= 28.5314 ZY= -1.5762

XZ= 0.3378 YZ= -0.9069 ZZ= 24.3020

Eigenvalues: 23.9240 27.3496 33.4820

42 H Isotropic = 27.8413 Anisotropy = 9.0561

XX= 28.5217 YX= 1.2586 ZX= 5.6787

XY= 1.3439 YY= 25.3382 ZY= -1.1956

XZ= 3.8048 YZ= -1.8658 ZZ= 29.6641

Eigenvalues: 22.7711 26.8742 33.8787

43 O Isotropic = 302.6285 Anisotropy = 47.8643

XX= 316.6984 YX= -9.9801 ZX= 0.0742

XY= -35.4362 YY= 305.2131 ZY= 1.4815

XZ= 14.0104 YZ= 7.6810 ZZ= 285.9739

Eigenvalues: 278.6996 294.6478 334.5380

44 H Isotropic = 27.2472 Anisotropy = 23.9929

XX= 37.2233 YX= -9.2047 ZX= -0.3594

XY= -9.5177 YY= 28.5530 ZY= 1.4512

XZ= -1.0716 YZ= 0.0922 ZZ= 15.9654

Eigenvalues: 15.9168 22.5824 43.2425

45 O Isotropic = 228.9602 Anisotropy = 99.9797

XX= 189.2033 YX= -34.1579 ZX= 19.1580

XY= -41.8091 YY= 245.4503 ZY= -29.1783

XZ= 18.3271 YZ= -34.0519 ZZ= 252.2271

Eigenvalues: 169.9723 221.2951 295.6134