PBLG as a Versatile Liquid Crystalline Medium for Anisotropic NMR Data Acquisition

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Supplemental Information

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Experimental

NMR experiments utilized for Residual Dipolar Coupling (RDC) and Residual Chemical Shift Anisotropy (RCSA) acquisition in PBLG liquid crystalline solutions have been previously reported.[1,2] RCSA measurements utilizing equation S1 require three ^{13}C NMR experiments – isotopic ^{13}C NMR without addition of poly-γ-benzyl-L-glutamate (PBLG), $\Delta\delta_{I0}$, isotropic ^{13}C NMR after addition of an amount of PBLG below its liquid crystal (LC) forming critical mass concentration, $\Delta\delta_{I1}$, and anisotropic ^{13}C NMR with an amount of PBLG above its LC forming critical mass concentration, $\Delta\delta_{A1}$.

$$RCSA = \Delta\delta_{A_1} - \Delta\delta_{I_0} - \frac{[P]_{A_1}}{[P]_{I_1}} * (\Delta\delta_{I_1} - \Delta\delta_{I_0}) \quad \text{S1}$$

RDC measurements, in contrast, required only two measurements – ^{13}C *J*-resolved experiments[2] in solutions containing no PBLG (isotropic condition) and in solutions containing PBLG above the LC forming critical mass concentration (anisotropic condition). RDC values, $^1D_{CH}$, were measured as the difference between anisotropic and isotropic coupling constants, $^1D_{CH} = {}^1T_{CH} - {}^1J_{CH}$.

PBLG solutions were rendered completely homogeneous in the NMR tubes by spinning the tube in a centrifuge, stopping the centrifuge to invert the tube after which the tube was centrifuged again. The process was repeated until a homogeneous solution was obtained. Typically four to five centrifugations were sufficient to afford a homogeneous solution.

All experiments were performed for this study using a Bruker Avance III 500 MHz spectrometer equipped with a 5 mm TXI Prodigy™ LN_2 cryogenically cooled probe at a probe temperature of 25 °C except for parthenolide data which was acquired on Bruker Avance III 600 MHz spectrometer equipped with a 5 mm TXI CryoProbe™.

Sample preparation and data acquisition

Strychnine: (1) **90:10 $CDCl_3$/DMSO solution** – 6.12 mg of strychnine was dissolved in 153 µL of $CDCl_3$ after which a 17 µL of DMSO-d_6 (Cambridge Isotope Laboratories) was added – giving a total solution of 170 µL. An 8 µL aliquot of tetramethylsilane (TMS) was added to the mixture for a chemical shift reference and the resulting mixture was then transferred to a 3 mm tube. The three ^{13}C NMR spectra required for RCSA measurements were acquired as follows; first, an isotropic ^{13}C spectrum (307 scan, 64K t1 points, 2s relaxation delay, total acquisition time, 16 mins) was recorded in the mixed solvent system without any PBLG added. A second isotropic ^{13}C spectrum (650 scan, 64K t1 points, 2s relaxation delay, total acquisition time, 34 mins) was recorded after the addition of 13.02 mg of PBLG. Finally, the anisotropic ^{13}C spectrum (2560 scan, 64K t1 points, 2s relaxation delay, total acquisition time, 2hr 15 mins) was recorded following the addition of a total of 23.57 mg of PBLG. The PBLG

solutions were centrifuged as described above to ensure homogeneous solutions after each addition. A ^{13}C *J*-resolved_BIRD experiment (*J*-resolved hereafter), 4 scan 19528*128 (t2*t1) given a total acquisition time of 23 mins with a 2s relaxation delay, was also acquired with the initial isotropic solution. Following the second PBLG addition, a second ^{13}C *J*-resolved experiment (40 scan 19528*128 (t2*t1) given a total acquisition time of 3hr 43 mins with a 2s relaxation delay) was acquired using the anisotropic solution – facilitating the measurement of RDCs as described previously.[2] **NOTE**: It is important to ensure that the solution is not saturated with the analyte prior to NMR acquisition. This situation can lead to precipitation of the analyte (upon the addition of PBLG) and thus a variation in the analyte concentration, which may introduce corresponding errors in the measured RCSAs.

(2) **80:20 $CDCl_3$/DMSO solution** – 4.67 mg of strychnine was dissolved in 136 µL of $CDCl_3$ after which a 34 µL of DMSO-d_6 was added – giving a total solution volume of 170 µL. An 8 µL aliquot of TMS was added to the sample as a chemical shift reference, after which the resulting solution was transferred to a 3 mm NMR tube. The three ^{13}C NMR experiments (137 scans and 7 mins, 341 scans and 18 mins, 1045 scans and 55 mins, respectively) required for the RCSA measurements were performed as described for the 90:10 $CDCl_3$/DMSO solution but with additions of a total of 11.82 and 27.03 mg of PBLG, respectively, for the second and third experiments. The PBLG solutions were centrifuged as described above to ensure homogeneous solutions.

(3) **70:30 $CDCl_3$/DMSO solution** – 6.5 mg of strychnine was dissolved in 420 µL of $CDCl_3$ after which a 180 µL of DMSO-d_6 was added – giving a total solution of 600 µL. A 10 µL aliquot TMS was added to the mixture for chemical shift reference. The three ^{13}C NMR experiments required for RCSA measurements were acquired as described for the 90:10 $CDCl_3$/DMSO solution but with additions of a total of 55.16 and 95.55 mg of PBLG, respectively, for the second and third experiments. The three ^{13}C NMR experiments were acquired with 186 scans, giving a time of 10 mins (64K t1 points), 367 scans of a total of 20 mins (64K t1 points) and 841 scans of 18 mins acquisition (64K t1 points), respectively. The PBLG solutions were centrifuged as described above to ensure homogeneous solutions. RDC values were determined from the isotropic and anisotropic ^{13}C *J*-resolved experiments (the latter containing 95.55 mg PBLG). Isotropic ^{13}C *J*-resolved experiment, 8 scans 11563*128 (t2*t1) given a total acquisition time of 42 mins with a 2s relaxation delay while anisotropic ^{13}C *J*-resolved experiment, 24 scans 11563*128 (t2*t1) given a total acquisition time of 2hr 6 mins with a 2s relaxation delay.

Parthenolide: A 6.4 mg weighed sample of parthenolide, **2** (see Figure S4), was dissolved in 420 µL of $CDCl_3$ after which 180 µL of DMSO-d_6 was added – giving a total solution volume of 600 µL. A 5 µL aliquot of TMS was added to the mixture as a chemical shift reference. The three ^{13}C NMR experiments required for RCSA measurements were acquired as described for strychnine but with 40.60 and a total of 93.49 mg of PBLG, respectively, for the second and third experiments. The three ^{13}C NMR experiments were acquired with 97 scans, giving a time of 5 mins (64K t1 points), 277 scans of

a total of 14 mins (64K t1 points) and 354 scans of 18 mins acquisition (64K t1 points), respectively. The PBLG solutions were centrifuged as described above to ensure homogeneous solutions. RDC values were determined from ^{13}C *J*-resolved experiments acquired with the isotropic solution and the anisotropic solution containing 93.49 mg PBLG). Isotropic ^{13}C *J*-resolved experiment was acquired with 2 scans of 19528*128 (t2*t1), given a total acquisition time of 12 mins with a 2s relaxation delay while anisotropic ^{13}C *J*-resolved experiment was acquired with 4 scans of 19528*128 (t2*t1), given a total acquisition time of 24 mins with a 2s relaxation delay.

Sucrose: 2.71 mg of sucrose, **3** (see Figure S6), was first dissolved in 180 µL of DMSO-d_6, gently applying heat until complete dissolution was achieved. The solution was allowed to cool to room temperature before the addition of 420 µL of $CDCl_3$ – giving a total solution of 600 µL. A 5 µL aliquot of TMS was added to the mixture for a chemical shift reference. The three ^{13}C NMR spectra were acquired for the RCSA measurements as described for strychnine (**1**) but with a total of 55.91 and 91.46 mg of PBLG added before the second and third spectra were acquired. The three ^{13}C NMR experiments were acquired with 301 scans, giving a time of 20 mins (64K t1 points), 502 scans of a total of 34 mins (64K t1 points) and 1535 scans of 1hr 44 mins acquisition (64K t1 points), respectively. The PBLG solutions were centrifuged as described above to ensure homogeneous solutions. RDC values were determined from ^{13}C *J*-resolved experiments acquired with the isotropic solution and the anisotropic solution containing 91.46 mg PBLG). Isotropic ^{13}C *J*-resolved experiment was acquired with 4 scans of 19528*128 (t2*t1), given a total acquisition time of 23 mins with a 2s relaxation delay while anisotropic ^{13}C *J*-resolved experiment was acquired with 32 scans of 19528*128 (t2*t1), given a total acquisition time of 3 hrs with a 2s relaxation delay.

Table S1: Strychnine RDC values measured in PBLG liquid crystalline solutions in $CDCl_3$, $CDCl_3$/DMSO (90:10) and $CDCl_3$/DMSO (70:30). $CDCl_3$ Residual Quadrupolar Coupling (RQC) values for each co-solvents mixture are shown.

Atom	Number of protons	RDC 100% $CDCl_3$ (Hz)	RDC 90:10 $CDCl_3$/DMSO (Hz)	RDC 70:30 $CDCl_3$/DMSO (Hz)
C3	1	-51.4	-76.99	-112.66
C22	1	0.7	5.32	15.89
C2	1	-	-	-39.77
C1	1	-135.5	-118.52	-60.45
C4	1	-135.5	-118.90	-63.43
C12	1	104.9	115.29	96.36
C16	1	-34.5	-35.59	-21.87
C8	1	67.5	72.82	96.63
C13	1	31.2	55.55	50.54
C14	1	114.7	-	74.48
C23	2	67.5	70.17	71.47
C20	2	28.3	36.81	54.4
C18	2	-22.6	-13.57	9.87
C17	2	-12.4	-	8.41
C11	2	15.5	34.19	68.89
C15	2	-35	-31.60	-27.31
RQC		215.5	198.2	134.6

Table S2: Strychnine RCSA values measured in PBLG liquid crystalline solutions in $CDCl_3$/DMSO (90:10), $CDCl_3$/DMSO (80:20) and $CDCl_3$/DMSO (70:30). $CDCl_3$ RQCs for the co-solvent mixtures are shown.

Atom	RCSA 100% $CDCl_3$ (Hz)	RCSA 90:10 $CDCl_3$/DMSO (Hz)	RCSA 80:20 $CDCl_3$/DMSO (Hz)	RCSA 70:30 $CDCl_3$/DMSO (Hz)
C10	26.8	24.89	27.36	27.79
C5	29.3	25.95	26.7	25.92
C21	34.9	20.12	10.68	3.02
C6	45.4	40.82	43.32	43.41
C3	52.2	48.51	54.31	54.82
C22	23.8	14.69	10.48	-0.62
C2	45.4	40.47	42.23	39.1
C1	67.2	54.87	52.83	45.61
C4	59.2	49.48	48.46	43.97
C12	1.8	0.43	0.3	0.35
C23	-6.2	-8.37	-14.91	-14.69
C16	-2.4	-3.56	-2.58	-1.87
C8	-14.3	-11.89	-12.31	-11.28
C20	1.3	-2.71	-3.5	-5.34
C7	-3.4	-3.5	-4.08	-4.4
C18	13.6	9.64	9.9	9.28
C13	0.4	-0.95	-0.91	-0.41
C17	6.4	4.84	5.27	5.96
C11	-4.7	-5.32	-8.87	-11.32
C14	2.8	2.05	2.22	3.16
C15	-6.7	-5.72	-5.38	-3.85
RQC	215.5	198.2	176.4	134.6

Table S3: Summary of orientation properties of strychnine, **1**, as a function of $CDCl_3$/DMSO co-solvent ratios. The mass of PBLG in each solution was above the LC forming critical mass concentration for the respective solvent or co-solvent system.

Parameters		RDC 100% CDCl3	RDC 90:10 CDCl3/DMSO	RDC 70:30 CDCl3/DMSO
Mass of PBLG (mg)		68.4[a]	95.55[a]	23.57[b]
No. of RDC		15	13	16
Q		0.034	0.060	0.039
Saupe order matrix ($*10^{-3}$)	S_{YY}	2.479	2.071	0.910
	S_{ZZ}	-2.813	-3.161	-3.448
	S_{XY}	1.027	0.902	0.621
	S_{YZ}	0.619	0.712	0.293
	S_{XZ}	-0.397	-0.069	0.573

[a]600 µL of solution [b]170 µL of solution

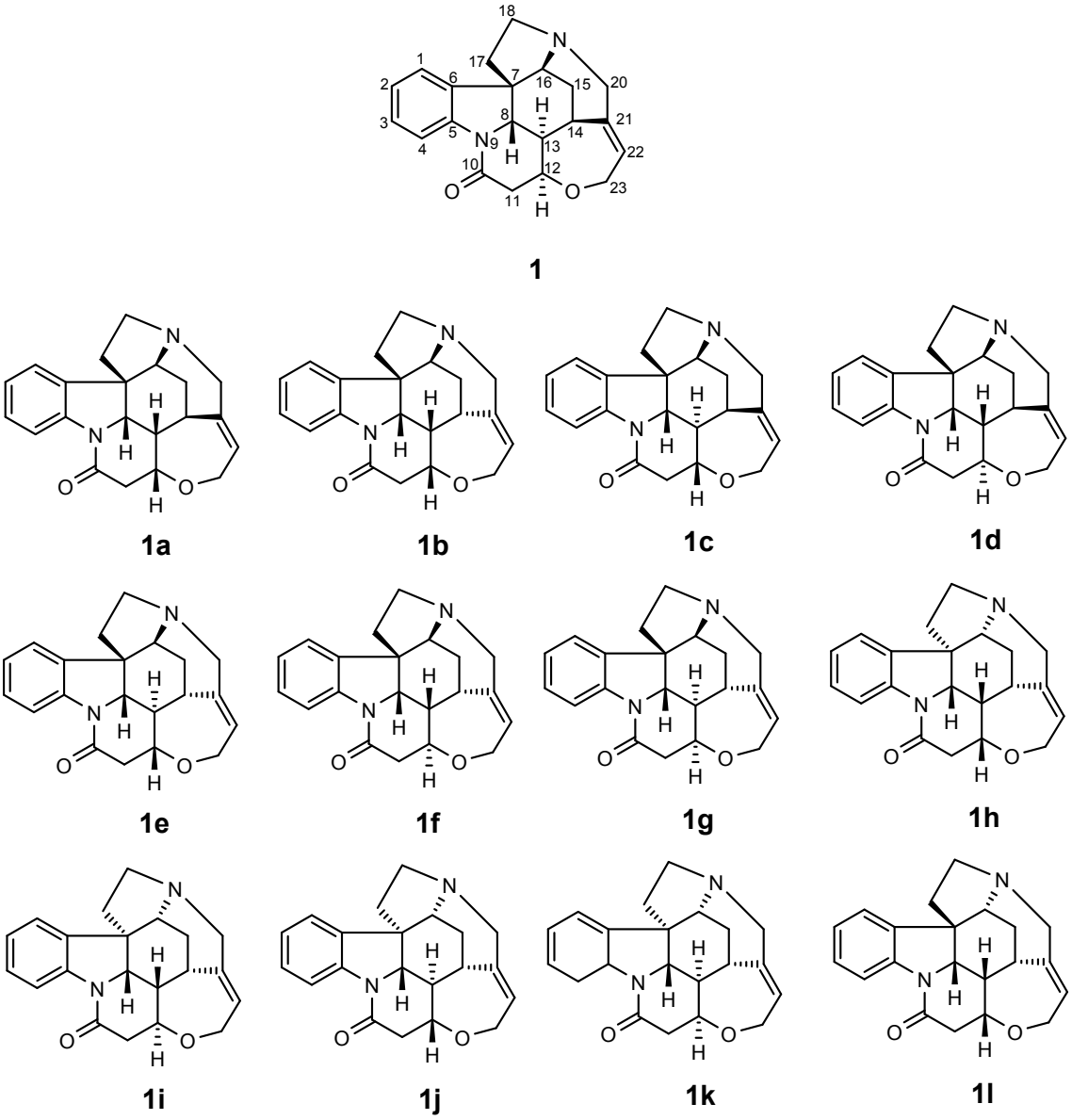

Figure S1. Structures of strychnine and its twelve structurally feasible diastereomers utilized for the SVD analysis with the measured RDC and RCSA values.

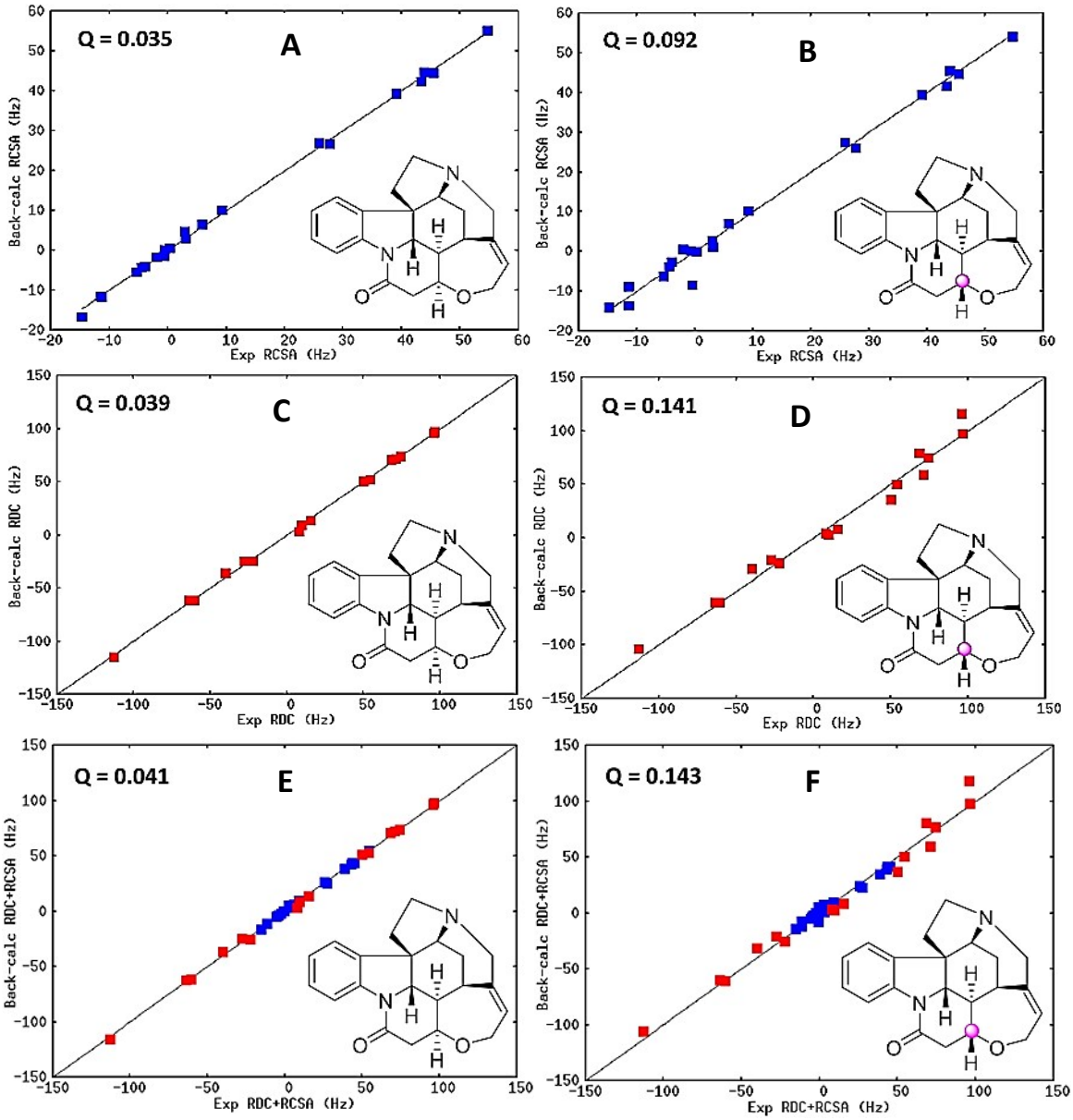

Figure S2. Stereochemical differentiation of strychnine and 12-*epi* strychnine (with the inverted stereocenter highlighted inset) using RCSA and RDC data acquired from the PBLG LLC solution in $CDCl_3$/DMSO-d_6 at 70:30. (A) and (B) are, respectively, strychnine and 12-*epi* strychnine plots of back calculated and experimental RCSA. (C) and (D) are RDC equivalent measured from the same solution and (E) and (F) are SVD analysis utilizing both RDC (red) and RCSA (blue) data in tandem.

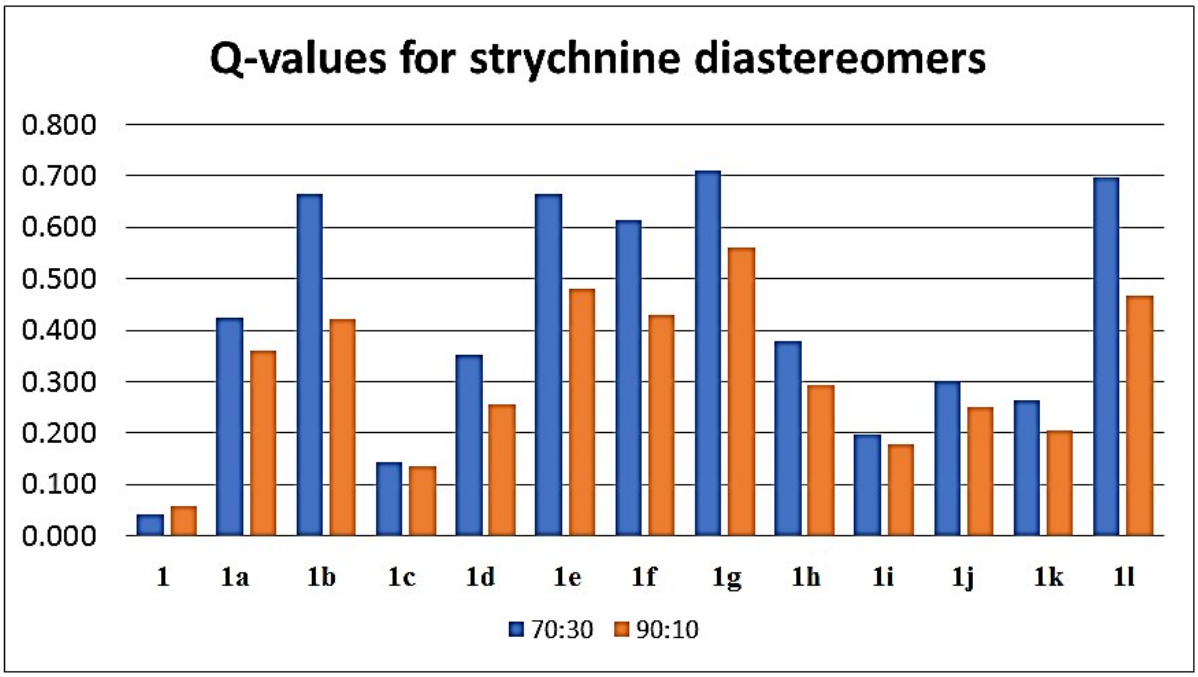

Figure S3. Histogram showing *Q*-values from the SVD analysis of strychnine, **1**, and its twelve structurally feasible diastereomers (see Figure S1), utilizing both RDC and RCSA values measured in $CDCl_3$/DMSO co-solvent systems of PBLG. Blue bars represent the *Q*-values for strychnine and its diastereomers using RDC and RCSA data from the 70:30 $CDCl_3$/DMSO solution while orange bars are *Q*-values derived from fitting to the 90:10 $CDCl_3$/DMSO solution (RDC/RCSA values in 100% $CDCl_3$ have already been published elsewhere[1,2]). The 70:30 co-solvent PBLG solution gave slightly better discrimination for strychnine and its diastereomers than the 90:10 co-solvent system. For instance, in the 70:30 co-solvent PBLG solution, the difference between the *Q*-value of strychnine, **1**, 0.041, and the nearest diastereomer, **1c**, 0.143, is **0.102**. This is substantially higher than the difference between the same pair of diastereomers (*Q*-values of 0.59 for **1** and 0.137 for **1c**) in the 90:10 co-solvent PBLG solution of **0.078**. This trend is also observed for other diastereomers as well.

Table S4. Table of *Q*-values for strychnine and its twelve diastereomers computed using RDC and RCSA values acquired in 100% $CDCl_3$, 90:10 $CDCl_3$/DMSO and 70:30 $CDCl_3$/DMSO PBLG solutions.

	100% CDCl3			90:10 CDCl3/DMSO			70:30 CDCl3/DMSO		
Isomers	RDC	RCSA	RDC/RCSA	RDC	RCSA	RDC/RCSA	RDC	RCSA	RDC/RCSA
1	0.034	0.032	0.038	0.060	0.051	0.086	0.039	0.035	0.070
1a	0.365	0.181	0.377	0.357	0.207	0.360	0.413	0.264	0.422
1b	0.435	0.186	0.443	0.382	0.203	0.411	0.681	0.255	0.658
1c	0.112	0.112	0.128	0.131	0.107	0.143	0.141	0.092	0.140
1d	0.203	0.153	0.222	0.236	0.181	0.247	0.336	0.250	0.342
1e	0.460	0.195	0.500	0.407	0.215	0.472	0.656	0.262	0.655
1f	0.444	0.211	0.475	0.374	0.216	0.418	0.614	0.284	0.606
1g	0.549	0.175	0.572	0.529	0.205	0.553	0.705	0.307	0.703
1h	0.325	0.136	0.321	0.286	0.148	0.283	0.395	0.171	0.373
1i	0.255	0.150	0.251	0.168	0.147	0.170	0.193	0.163	0.199
1j	0.244	0.120	0.261	0.239	0.128	0.244	0.297	0.179	0.292
1k	0.258	0.118	0.253	0.201	0.126	0.195	0.272	0.143	0.257
1l	0.384	0.194	0.387	0.463	0.238	0.456	0.719	0.374	0.689

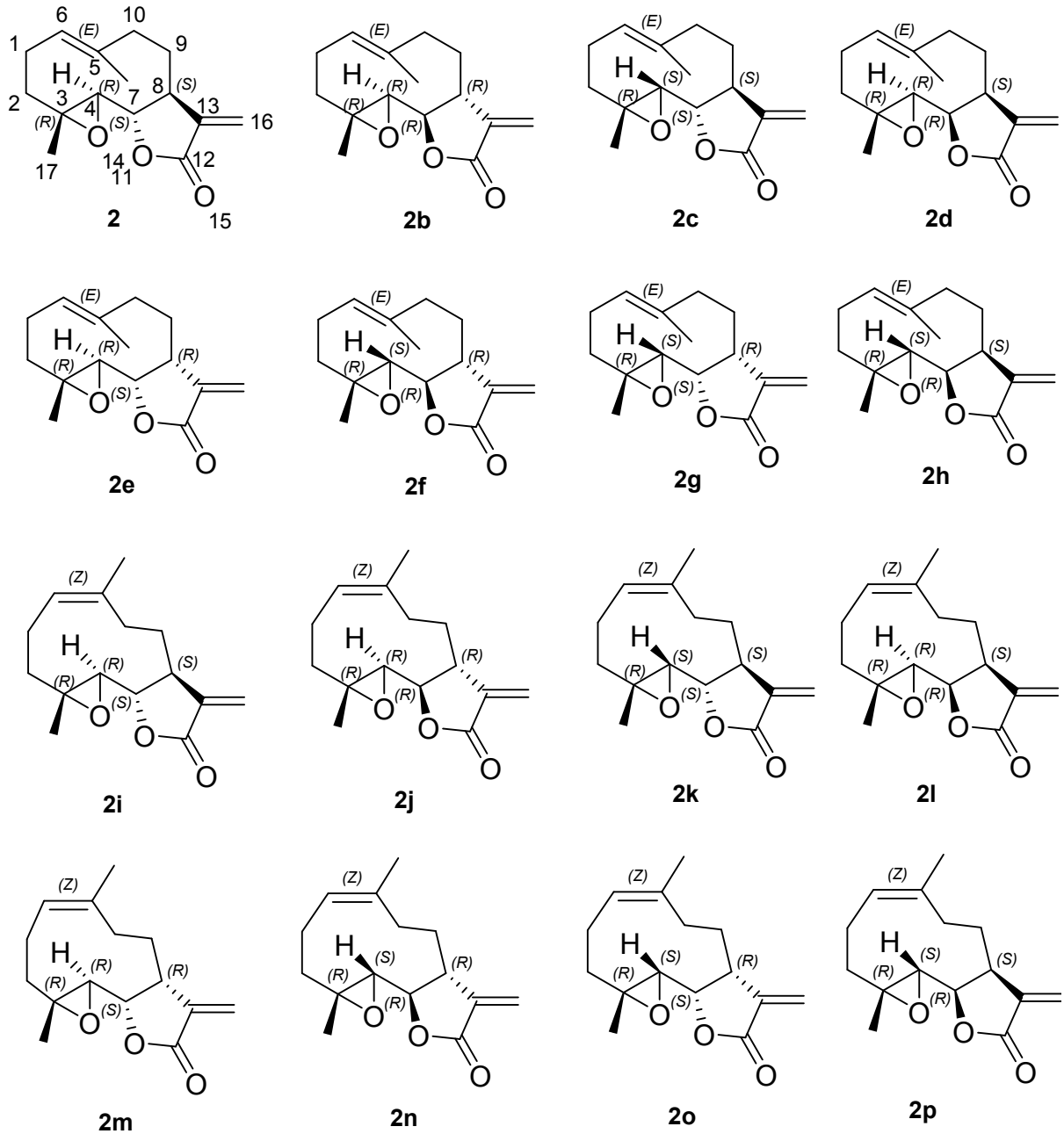

Figure S4. Structures of parthenolide and fifteen diastereoisomers utilized for SVD analysis with the measured RDC and RCSA values. DFT structures and tensors were derived with GIAO-mPW1PW91[7]/6-311+G(2d,p)//M06-2X[8]/6-31+g(d,p).

Table S5. RDC and RCSA values of parthenolide acquired in the $CDCl_3$/DMSO (70:30) PBLG LLC solution. $CDCl_3$ RQC is also shown.

Atom	Number of protons	RDC (Hz)	RCSA (Hz)
C12	-	-	9.77
C13	-	-	32.76
C5	-	-	-1.31
C6	1	31.84	-3.12
C16	2	-57.18	40.76
C7	1	-	-13.16
C4	1	94.72	12.61
C3	-	-	13.40
C8	1	112.82	-1.47
C10	2	31.08	-1.74
C2	2	15.7	4.24
C9	2	24.4	-2.93
C1	2	43.7	-4.99
C17	3	-23.75	5.63
C18	3	-14.17	-0.52
RQC		126.9	

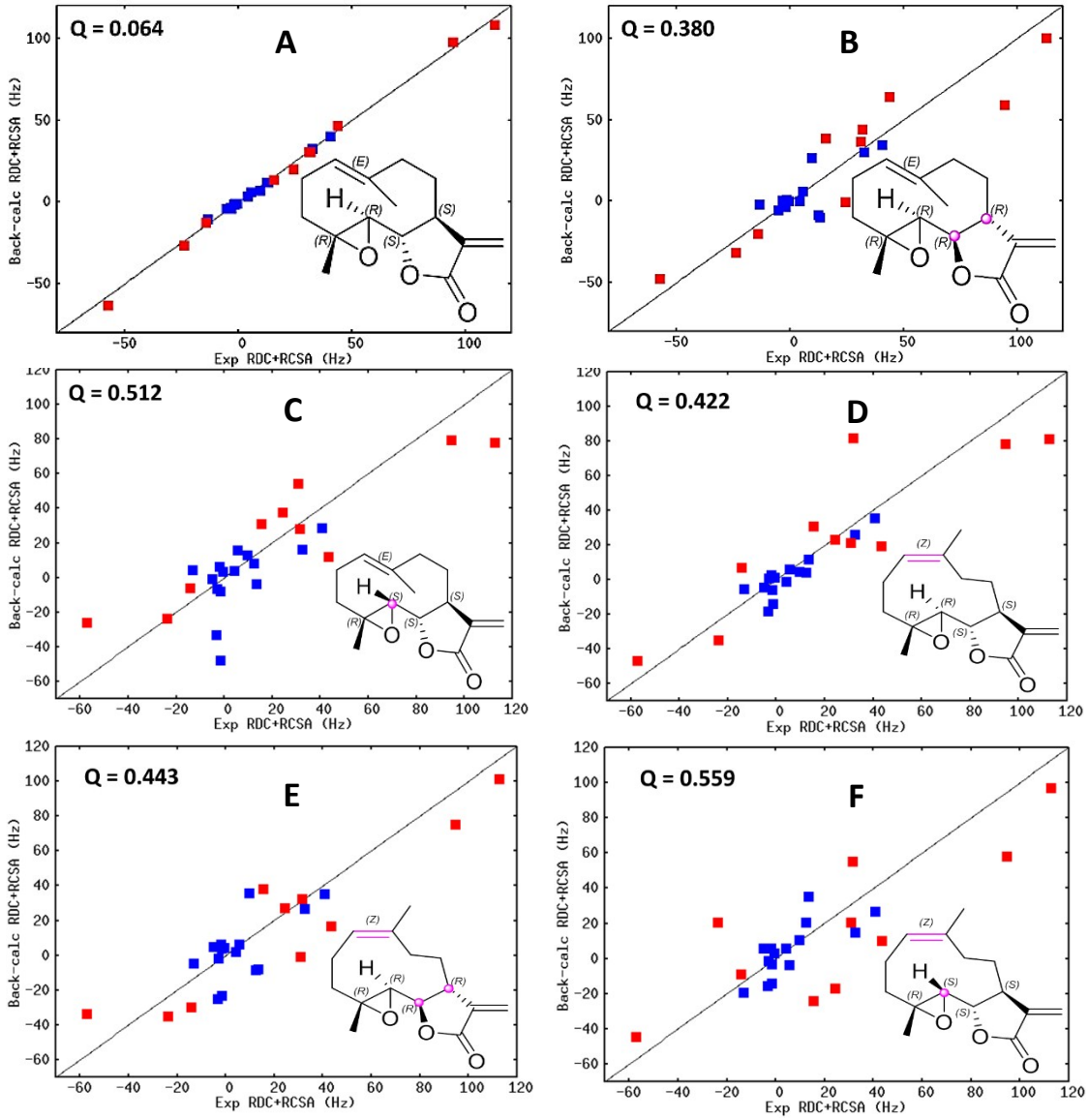

Figure S5. Back-calculated *vs*. experimental RDC (red) and RCSA (blue) plots of isomers of parthenolide obtained from SVD fitting protocol for (A) parthenolide – *RRSSE* – and its isomers (B) *RRRRE*, (C) *RSSSE*, (D) *RRSSZ*, (E) *RRRRZ* and (F) *RSSSZ*, with the inverted stereochemistry shown inset.

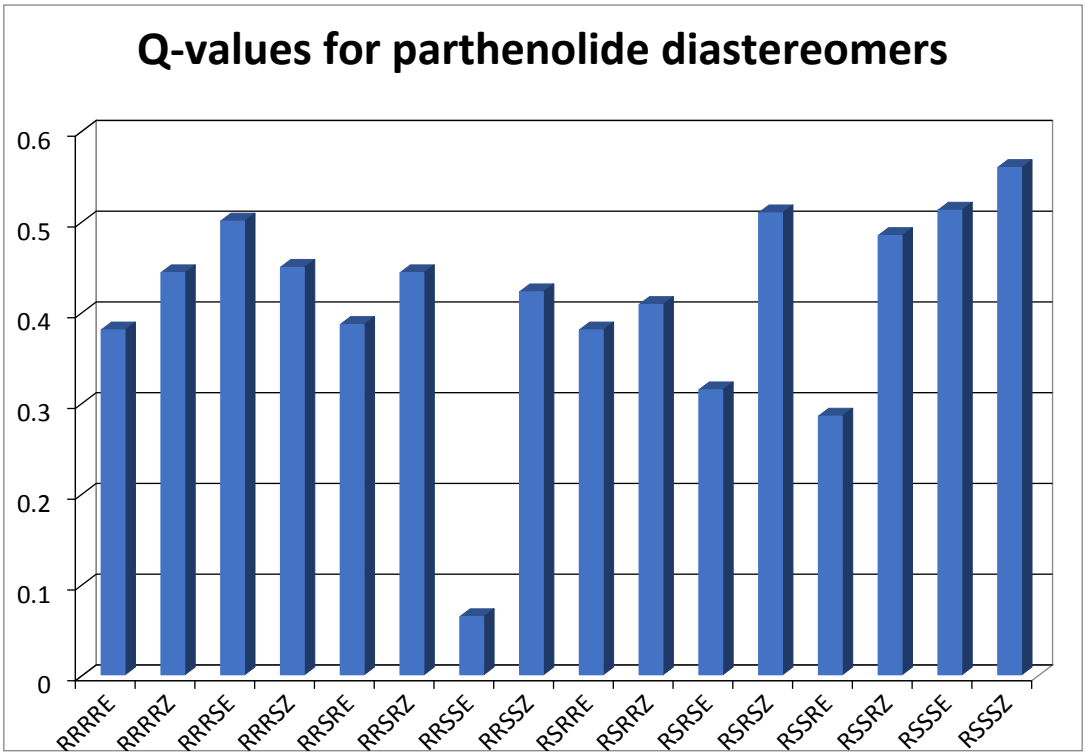

Figure S6. Histogram showing *Q*-values from the SVD analysis of parthenolide, **2**, and its fifteen diastereomers (see Figure S4), utilizing both RDC and RCSA values measured in $CDCl_3$/DMSO co-solvent solutions of PBLG.

Table S6. Table showing Q-values computed for parthenolide diastereomers using RDC and RCSA data acquired in 70:30 $CDCl_3$/DMSO.

Q-values of parthenolide isomers			
Isomers	RDC	RCSA	RDC/RCSA
RRRRE	0.329	0.250	0.380
RRRRZ	0.334	0.478	0.443
RRRSE	0.433	0.306	0.500
RRRSZ	0.376	0.631	0.449
RRSRE	0.343	0.200	0.386
RRSRZ	0.429	0.284	0.443
RRSSE	0.061	0.049	0.064
RRSSZ	0.414	0.291	0.422
RSRRE	0.379	0.167	0.380
RSRRZ	0.386	0.153	0.408
RSRSE	0.315	0.093	0.314
RSRSZ	0.462	0.380	0.509
RSSRE	0.284	0.191	0.285
RSSRZ	0.442	0.540	0.484
RSSSE	0.343	0.212	0.512
RSSSZ	0.525	0.153	0.559

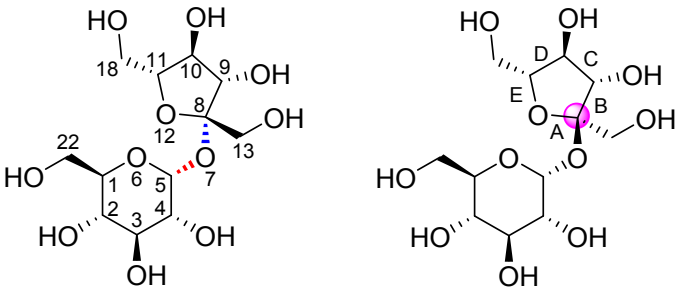

Figure S7. Structures of sucrose and its diastereomer, 2′-*epi* sucrose, utilized for SVD analysis with the measured RDC and RCSA values. φ Represents dihedral angles for sucrose measured as a function of rotations around the red hashed bond whereas ψ dihedral angles relate to rotations around blue hashed bond. Labels A, B, C, D, and E indicate bonds about which dihedral angles θ_0, θ_1, θ_2, θ_3, and θ_4 (in degrees), respectively, of the fructosyl units were measured.

Sucrose Conformational Modelling

Previous studies[3–5] on the solution structure of sucrose, established four free energy wells on the potential energy surface (PES) as determined with molecular dynamic simulations. The clusters, M1-M4, consist of conformers of similar dihedral angles around the glycosidic linkage (φ, ψ) (**Fig. S6**) – within a 20° radius. The four free energy wells were determined as M1 (104.5, 306.1), M2 (69.7, 283.3), M3 (88.5, 195.9) and M4 (92.9, 54.3).[3] Furthermore, the fructosyl pucker phase, P, was determined to favour the north-east (NE) quadrant of the pseudo-rotation wheel – with a formalism described (equation S2) for calculating the fructosyl conformation based on the five dihedral angles, θ_0, θ_1, θ_2, θ_3, and θ_4 (see **Fig. S6** and caption for details).[6] Sucrose conformations from DFT calculations (GIAO-mPW1PW91[7]/6-311+G(2d,p)//M06-2X[8]/6-31+g(d,p)) in implicit DMSO with the solvation model density (SMD) method – after exhaustive conformational search in Spartan 16 utilizing MMFF energy cutoff of 15 kcal/mol – were classified into the four aforementioned M-clusters, and those conformations within 8 kcal/mol Gibbs free energy are listed in **Table S5**. In addition, the fructosyl pucker phase was calculated using the Altona and Sundaralingam equation (equation S2) as well as the correction factor specified (adding 180° to calculated P values for all negative θ_2 (see **Table S5-S7**).[6] As shown in Table S5, conformations with the lowest theoretical energies all fall into the M1 cluster, whereas the valleys of the M2, M3, and M4 clusters are over 4 kcal/mol higher in energy relative to the M1 valley. It is also noted that fructosyl pucker of the lowest energy conformations favors the NE and SW quadrants[6] of the pseudo-rotation wheel (**Table S5**). In Table S6, conformations with similar fructosyl pucker phases are labeled with the same color in each M-cluster. It is worth noting that the pucker phase has a period of 360°, and therefore a phase of 357°, for example, is considered similar to a phase of 3°, with a 6° difference.

$$\tan P = \frac{(\theta_4 + \theta_1) - (\theta_3 + \theta_0)}{2\theta_2(\sin 36 + \sin 72)} \qquad \text{S2}$$

Single-tensor SVD Analysis of Sucrose with both RDC and RCSA data

Initial SVD analysis of selected sucrose conformers, constituting about ~1% Boltzmann distribution and higher, revealed the need for ensemble averaging since individual conformations did not fully describe the experimental data (**Table S7**) – as evidenced by the appreciably high Q-factors derived for each (see main paper). Ensemble averaging utilizing variable-weight single-tensor SVD method,[9–11] with four conformers from M1 (highlighted in red in **Table S5**) gave an improved Q-value of 0.061. A heavy-atom superposition of the selected conformers is shown in **Fig. S9a**. Similarly, low-energy conformers from M2, M3 and M4 that represent major fructosyl conformations (highlighted in red in

corresponding sections of Table S5) were also fitted to the measured RDC/RCSA data through the same SVD analysis procedure. Significantly higher Q-values of 0.245, 0.371 and 0.396, respectively, for M2, M3 and M4 were obtained, as reported in the main text. These high values indicate that these clusters do not describe the experimentally measured data and are thus unlikely to represent major sucrose conformation in the $CDCl_3$/DMSO-d_6 mixture utilized to acquire the data. In contrast, a similar SVD fitting of the same selected set of low-energy conformers from the four clusters to previously reported RDC data acquired in water-d_2,[5] was non-discriminatory with Q-values of 0.231, 0.221, 0.245 and 0.205, respectively, for M1, M2, M3 and M4 clusters, supporting the conclusion from earlier studies that molecules in aqueous solutions of sucrose undergo significant conformational exchange across different M-clusters. To further evaluate potential solvation effects on sucrose conformational distribution, we re-optimized selected sucrose conformers (GIAO-mPW1PW91[7]/6-311+G(2d,p)//M06-2X[8]/6-31+g(d,p)) in implicit water using SMD model. The results, as listed in **Table S6,** clearly show a reduction in the inter-cluster energy barrier between M1 and the other three clusters when compared to calculations in DMSO. Based on the foregoing, we can conclude that sucrose is somewhat less flexible in chloroform/DMSO solution – involving mostly small conformational variations at the glycosidic linkage within M1 – albeit with significant fructosyl ring pucker changes. Conversely, sucrose becomes more flexible in water with high amplitude conformational exchange across different M-clusters.

In the same vein, five representative conformers were selected for the 2′-*epi* sucrose (labelled in red in **Table S7**), and analysed by single-tensor SVD analysis for stereochemical differentiation. A heavy-atom superposition of selected conformers is shown in **Fig. S9b**. SVD single-tensor analysis with the measured RDC and RCSA data gave a substantially higher *Q*-value of 0.320 (compared to 0.061 for sucrose), providing crucial evidence that this approach can be utilized for facile stereochemical differentiation.

Table S7. Table showing selected conformers of sucrose clusters, M1-M4, sorted based on their DFT energies in implicit DMSO solvent, ΔG (M06-2X[8]/6-31+g(d,p)), glycosidic dihedral angles, φ and ψ, as well as the fructosyl pucker phase, P (derived from equation S2).[6]

Sucrose											
Cluster	Conformer	ΔG (Kcal/mol)	ϕ	Ψ	Pucker phase, P	Fructosyl dihedral angle					Cal. P
						A	B	C	D	E	
M1 (104.5, 306.1)	**Sucrose_4.out**	0	107.33	318.54	2.83	11.2434	-32.7581	40.4788	-34.9281	15.2335	2.830774
	Sucrose_1.out	1.228663	98.37	334.42	11.35	5.1708	-28.6043	39.7746	-37.6033	20.7331	11.34529
	Sucrose_17.out	1.450173	104.57	321.53	6.72	8.4379	-30.4041	39.8015	-35.7823	17.4828	6.715261
	Sucrose_153.out	2.044424	104.71	318.83	219.96	13.1815	9.7192	-27.009	35.3772	-30.8145	39.96103
	Sucrose_122.out	2.717114	109.39	310.87	356.93	14.5242	-33.474	38.4525	-31.0228	10.6189	-3.0745
	Sucrose_12.out	3.000748	103.87	317.62	221.33	13.7576	8.7529	-26.1011	34.737	-30.8931	41.32509
	Sucrose_5.out	3.306345	103.97	326.75	7.75	7.3291	-28.6714	37.9354	-34.521	17.362	7.746672
	Sucrose_3.out	3.3327	111.06	307.24	353.63	17.012	-35.5627	39.3773	-30.478	8.5765	-6.36566
	Sucrose_265.out	3.488323	104.15	318.07	221.89	14.0553	8.3928	-25.8199	34.601	-31.0052	41.88738
	Sucrose_392.out	3.549818	103.45	326.90	7.37	7.6166	-28.9854	38.1546	-34.573	17.2086	7.365638
	Sucrose_79.out	3.638925	103.45	318.58	221.48	13.8711	8.6732	-26.0761	34.7665	-30.982	41.47743
	Sucrose_336.out	3.639552	103.45	318.32	221.24	13.7432	8.8195	-26.1818	34.8024	-30.9271	41.2448
	Sucrose_10.out	3.719873	106.02	324.46	219.57	13.1247	10.0582	-27.5234	35.8533	-31.0799	39.56902
	Sucrose_423.out	3.775094	104.45	318.08	221.70	14.1884	8.6645	-26.2589	35.1495	-31.3256	41.69765
	Sucrose_92.out	3.837845	103.17	318.81	220.26	13.3694	9.5465	-26.8989	35.3555	-30.9199	40.25585
	Sucrose_134.out	3.896203	103.31	319.61	221.22	13.7423	8.8345	-26.2326	34.8588	-30.9606	41.21948
	Sucrose_204.out	3.910636	106.82	314.89	206.49	4.3573	15.294	-27.706	31.0506	-22.3819	26.4901
	Sucrose_242.out	3.911264	97.93	324.29	12.38	4.2981	-27.442	38.6509	-36.9436	20.9052	12.37918
	Sucrose_30.out	3.918794	105.43	315.58	204.99	3.4432	15.8041	-27.7926	30.6272	-21.6093	24.99401
	Sucrose_84.out	3.927579	107.84	317.60	209.83	6.1593	13.6129	-26.8294	31.1368	-23.6729	29.8347
	Sucrose_239.out	3.934481	108.35	316.04	207.94	5.087	14.4436	-27.1459	30.8522	-22.8067	27.93572
	Sucrose_455.out	3.988447	93.82	327.84	211.29	7.6841	14.2518	-28.9508	34.0451	-26.6731	31.28873

	Sucrose_38.out	4.013548	98.74	334.45	357.52	13.8687	-32.4197	37.6422	-30.5175	10.747	-2.48309
	Sucrose_426.out	4.017313	104.09	318.44	221.02	13.803	9.0716	-26.5394	35.2173	-31.1166	41.02479
M2 (69.7, 283.3)	**Sucrose_233.out**	4.752126	63.45	274.99	352.63	16.7245	-34.2329	37.298	-28.6069	7.503	-7.36991
	Sucrose_44.out	4.929083	73.77	287.35	28.50	-7.4256	-19.2583	36.8561	-42.0112	31.4176	28.50307
	Sucrose_116.out	5.577928	73.30	287.91	30.51	-8.9221	-18.1674	36.3017	-42.5007	32.5702	30.50551
	Sucrose_166.out	5.666406	72.16	287.74	26.84	-6.2332	-20.5477	37.6105	-42.0964	30.7967	26.84236
	Sucrose_64.out	5.819518	62.08	284.76	212.40	7.4998	12.0701	-25.5549	30.3643	-24.1213	32.40133
	Sucrose_199.out	6.209202	63.05	277.41	358.91	13.4428	-33.319	39.4678	-32.4396	12.0189	-1.08631
	Sucrose_190.out	6.587589	63.97	281.97	213.76	8.2538	11.6128	-25.4148	30.7853	-24.8651	33.76384
	Sucrose_97.out	6.699914	60.97	285.12	211.45	6.7978	12.1682	-25.0706	29.4668	-23.0944	31.45002
	Sucrose_290.out	6.769567	59.44	272.65	349.06	19.1672	-35.4289	37.6398	-27.1978	5.014	-10.9364
	Sucrose_163.out	6.962212	63.62	281.20	213.65	8.1835	11.6642	-25.4304	30.765	-24.8073	33.64635
	Sucrose_144.out	7.113442	61.89	284.89	19.85	-1.0369	-23.9525	38.3126	-39.5939	25.887	19.84886
	Sucrose_216.out	7.149838	63.45	284.54	210.74	6.6477	12.8768	-26.1165	30.5125	-23.5256	30.74417
	Sucrose_209.out	7.242709	72.49	288.94	32.06	-9.998	-17.1195	35.7264	-42.5673	33.4322	32.06395
	Sucrose_234.out	7.257769	67.74	269.52	346.50	20.4468	-35.9007	36.9112	-25.6879	3.3816	-13.5023
	Sucrose_370.out	7.294165	58.97	290.49	175.38	-11.6547	25.8086	-29.0913	22.9847	-7.2378	-4.62358
	Sucrose_48.out	7.409626	66.14	286.81	206.31	4.0742	14.4904	-26.4641	29.4418	-21.2436	26.3085
	Sucrose_149.out	7.576544	65.19	284.44	206.12	3.8826	14.4227	-26.081	29.0203	-20.8728	26.11703
	Sucrose_66.out	7.651217	66.32	286.76	206.79	4.4044	14.428	-26.5639	29.7382	-21.5609	26.78768
	Sucrose_331.out	7.702673	71.09	274.33	5.97	8.6781	-29.9018	38.1617	-34.4982	16.373	5.974352
	Sucrose_186.out	7.710831	65.51	284.35	206.95	4.3906	14.1997	-26.094	29.3282	-21.3138	26.95092
	Sucrose_316.out	7.817507	63.55	281.60	214.01	8.3793	11.4899	-25.3352	30.7779	-24.9424	34.00796
	Sucrose_206.out	7.914771	63.34	283.46	218.45	11.49	9.5925	-25.4103	32.3681	-27.825	38.44775
M3 (88.5, 195.9)	**Sucrose_7.out**	4.542538	89.32	197.77	204.07	3.0789	16.7595	-28.9599	31.5453	-21.9498	24.07053
	Sucrose_15.out	4.590856	95.71	204.03	339.23	23.9794	-36.1789	34.4699	-21.4788	-1.5563	-20.7702
	Sucrose_8.out	4.72326	85.65	186.22	219.82	12.9608	9.6316	-26.6365	34.6969	-30.3246	39.82005

	Sucrose_25.out	4.773461	91.81	202.63	339.17	23.5556	-35.2818	33.6671	-21.0103	-1.603	-20.8337
	Sucrose_2.out	4.877	86.03	186.10	220.85	13.9127	9.2546	-26.89	35.4683	-31.4409	40.85222
	Sucrose_35.out	4.932848	93.56	193.25	323.16	28.021	-33.3437	26.4861	-11.1221	-10.8385	-36.8448
	Sucrose_6.out	4.935986	89.39	197.77	204.14	3.1819	16.8711	-29.1025	31.7543	-22.0665	24.13505
	Sucrose_191.out	4.937868	86.61	192.78	238.69	21.6815	-1.709	-16.9632	29.5737	-32.8538	58.68577
	Sucrose_19.out	5.145574	85.88	186.12	220.40	13.6421	9.5287	-27.0707	35.5034	-31.289	40.39966
	Sucrose_188.out	5.175067	83.34	185.64	224.31	16.1424	7.1963	-25.747	35.5166	-32.8862	44.30768
	Sucrose_173.out	5.19954	90.82	202.59	339.90	23.2762	-35.6329	34.2453	-21.4742	-1.1445	-20.1047
	Sucrose_16.out	5.286763	91.56	192.83	155.45	-22.585	32.1323	-29.2456	17.1129	3.5155	-24.553
	Sucrose_82.out	5.42858	84.91	188.53	227.67	18.2538	5.1018	-24.4752	35.326	-34.2063	47.6659
	Sucrose_18.out	5.522707	91.00	202.49	338.75	23.7145	-35.6012	33.7791	-20.7603	-1.8754	-21.2512
	Sucrose_13.out	5.530237	85.19	186.36	220.70	13.8371	9.3602	-26.9824	35.5249	-31.4264	40.69988
	Sucrose_63.out	5.625618	83.02	183.94	221.18	13.1781	8.4713	-25.1264	33.3461	-29.6059	41.18344
	Sucrose_175.out	5.809478	85.41	188.93	228.04	18.7077	4.9403	-24.5464	35.6472	-34.6014	48.03855
	Sucrose_335.out	5.854659	90.65	202.70	339.91	23.4228	-35.6894	34.3548	-21.5743	-1.1265	-20.0864
	Sucrose_65.out	5.886034	91.64	202.35	322.84	30.8438	-36.5986	28.8798	-12.0326	-11.9466	-37.1552
M4 (92.9, 54.3)	**Sucrose_288.out**	5.817008	92.29	49.90	14.49	2.5297	-24.0069	34.8524	-34.0214	20.2305	14.48737
	Sucrose_169.out	6.986685	101.37	39.88	174.63	-10.7643	22.9058	-25.6497	20.1994	-6.0561	-5.36577
	Sucrose_461.out	7.003628	90.30	45.78	14.86	2.4745	-25.4618	36.5934	-36.2146	21.6001	14.85807
	Sucrose_198.out	7.093989	100.19	43.17	171.95	-13.7652	26.806	-29.2312	22.3561	-5.486	-8.05335

Table S8. Table showing selected conformers of sucrose clusters, M1-M4, sorted based on their DFT energies in implicit water, ΔG (M06-2X[8]/6-31+g(d,p)), glycosidic dihedral angles, φ and ψ, as well as the fructosyl pucker phase, P (derived from equation S2).[6]

Sucrose											
						Fructosyl dihedral angle					
Cluster	Conformer	ΔG (Kcal/mol)	ϕ	Ψ	Pucker phase, P	A	B	C	D	E	Cal. P
M1 (104.5, 306.1)	Sucrose_4.out	0	105.54	322.03	4.17	10.2116	-31.7886	40.2117	-35.0963	15.936	4.174127
	Sucrose_17.out	0.200803	106.32	321.96	4.69	9.7674	-31.1303	39.6688	-34.8703	16.0436	4.690089
	Sucrose_122.out	0.450551	109.80	312.28	358.31	13.4814	-32.4573	38.1195	-31.1753	11.3081	-1.68699
	Sucrose_84.out	1.463351	107.13	316.41	209.88	6.1358	13.256	-26.3463	30.471	-23.233	29.87744
	Sucrose_3.out	1.464606	112.26	306.47	353.49	16.7131	-34.7164	38.5051	-29.6818	8.2336	-6.50572
	Sucrose_1.out	1.483431	99.12	334.13	10.26	5.8911	-28.9465	39.6818	-37.0413	19.9043	10.26075
	Sucrose_336.out	1.707452	106.49	317.23	227.12	17.2229	5.2257	-23.8752	34.2973	-32.8408	47.12206
	Sucrose_238.out	1.73318	96.59	327.20	214.67	9.9209	12.5763	-28.485	34.7756	-28.5086	34.66673
	Sucrose_92.out	1.792793	107.36	318.34	229.70	18.4918	3.6342	-22.4763	33.5604	-33.1467	49.69876
	Sucrose_204.out	1.801578	106.10	314.44	209.32	5.8673	13.5455	-26.4625	30.4348	-22.9779	29.31643
	Sucrose_239.out	1.809736	105.76	314.59	206.38	4.2409	14.8976	-27.198	30.2785	-21.8954	26.38065
	Sucrose_438.out	2.112195	110.40	317.42	0.07	12.9541	-33.4998	40.3213	-33.4454	13.1562	0.068194
	Sucrose_455.out	2.166161	96.57	327.12	214.61	9.8831	12.6032	-28.4903	34.762	-28.4754	34.61243
	Sucrose_392.out	2.312371	103.26	327.38	7.99	7.1471	-28.6342	38.0641	-34.674	17.5593	7.994123
	Sucrose_30.out	2.330568	105.32	315.60	208.58	5.4255	13.847	-26.6249	30.3562	-22.7101	28.58276
	Sucrose_38.out	2.457953	96.23	337.71	0.08	12.3453	-31.7986	38.1365	-31.8046	12.4956	0.076299
	Sucrose_265.out	2.47364	108.08	316.29	227.78	17.6461	4.8486	-23.6787	34.3486	-33.1573	47.77618
	Sucrose_153.out	2.700171	108.03	318.24	226.58	17.2625	5.6953	-24.5713	35.0674	-33.2817	46.58123
	Sucrose_79.out	2.730919	106.01	317.41	226.22	16.9048	5.842	-24.5501	34.8157	-32.9644	46.219
	Sucrose_426.out	2.748489	108.23	316.07	228.64	18.1767	4.3404	-23.2844	34.2341	-33.3398	48.64388
	Sucrose_5.out	2.810613	104.74	326.23	7.00	7.7941	-28.9788	37.9874	-34.2523	16.8812	7.002638
	Sucrose_12.out	2.810613	107.23	316.89	226.81	17.1023	5.4463	-24.1049	34.4823	-32.8906	46.80995

	Sucrose_423.out	2.892816	108.39	315.68	229.24	18.3736	3.9469	-22.8554	33.9024	-33.265	49.23561
	Sucrose_395.out	3.227279	106.39	307.53	315.31	29.6211	-32.276	22.9893	-6.5787	-14.6766	-44.6911
	Sucrose_134.out	3.392314	107.36	318.78	227.71	17.5927	4.8824	-23.6937	34.3328	-33.1173	47.70729
	Sucrose_28.out	3.487695	109.43	304.32	311.82	32.1296	-33.7612	22.8081	-4.8446	-17.4094	-48.1802
	Sucrose_10.out	3.643317	107.64	321.61	225.76	16.6116	6.1304	-24.6749	34.79	-32.7027	45.75651
	Sucrose_112.out	3.697283	103.95	308.22	318.54	28.4234	-32.2056	24.0044	-8.2005	-12.8495	-41.4636
	Sucrose_262.out	4.560108	108.79	318.72	342.65	23.7064	-38.1728	37.6104	-24.8619	0.864	-17.3452
	Sucrose_169.out	5.76618	95.95	354.38	179.54	-8.7166	21.8671	-26.0591	21.6743	-8.2587	-0.46485
	Sucrose_67.out	7.99823	97.63	194.01	333.60	27.3026	-37.9014	33.8777	-18.8526	-5.4019	-26.3981
M2 (69.7, 283.3)	Sucrose_75.out	2.343119	78.52	284.59	19.81	-0.951	-24.0742	38.3448	-39.7424	25.8912	19.80991
	Sucrose_233.out	2.389554	66.66	276.72	354.58	15.5484	-33.5861	37.6141	-29.4177	8.7273	-5.42284
	Sucrose_166.out	3.209081	80.43	286.02	17.54	0.673	-25.8016	39.4843	-39.8935	24.9833	17.53732
	Sucrose_116.out	4.154737	77.02	282.65	20.64	-1.6525	-24.4903	39.4699	-41.3353	27.2682	20.64376
	Sucrose_44.out	4.497985	75.85	281.48	20.03	-1.1601	-24.5499	39.2935	-40.7656	26.7065	20.02773
	Sucrose_64.out	4.684355	62.09	283.03	214.11	8.4142	11.145	-24.9915	30.2075	-24.6158	34.10843
	Sucrose_149.out	4.7333	67.59	282.27	212.23	7.2402	11.8571	-25.1455	29.852	-23.5546	32.22898
	Sucrose_48.out	4.829309	63.93	283.96	210.19	6.2619	12.91	-25.9672	30.0724	-23.0636	30.18609
	Sucrose_209.out	4.855037	78.38	281.67	18.47	0.0288	-25.3917	39.4746	-40.3409	25.6698	18.47459
	Sucrose_186.out	4.907748	67.70	282.14	213.02	7.7256	11.5791	-25.05	30.0287	-23.9254	33.01771
	Sucrose_66.out	5.323786	63.87	283.73	211.63	7.1332	12.3789	-25.8423	30.4417	-23.7865	31.62748
	Sucrose_172.out	7.135405	72.90	271.84	356.50	15.1343	-34.5785	39.612	-31.7201	10.5386	-3.49886
M3 (88.5, 195.9)	Sucrose_15.out	3.455065	94.56	200.29	336.07	25.3031	-36.252	33.4208	-19.5722	-3.6577	-23.9279
	Sucrose_7.out	4.03551	85.82	188.76	227.30	16.8001	4.9307	-22.9931	33.0447	-31.7675	47.29768
	Sucrose_6.out	4.422683	85.74	188.79	228.23	17.3678	4.4231	-22.6362	33.0024	-32.0407	48.22536
	Sucrose_16.out	4.775343	91.32	192.37	160.35	-19.2389	29.619	-28.4834	18.2392	0.6821	-19.6495

	Sucrose_43.out	4.946653	84.32	187.82	221.79	13.6131	8.0856	-24.8962	33.1581	-29.795	41.78839
	Sucrose_168.out	5.045172	92.25	187.03	151.69	-24.2243	32.4438	-28.4067	15.267	5.6982	-28.3126
	Sucrose_20.out	5.566005	84.61	188.56	222.00	13.666	7.922	-24.6885	32.9694	-29.7118	42.00393
	Sucrose_211.out	5.800693	89.24	194.44	240.38	27.101	-3.2204	-19.563	35.4326	-40.1512	60.38111
	Sucrose_158.out	5.913645	92.40	188.61	155.43	-22.1789	31.5149	-28.7228	16.7666	3.4908	-24.5708
	Sucrose_241.out	6.564999	87.87	181.16	142.30	-30.4065	36.1706	-28.2084	11.4817	11.9943	-37.696
	Sucrose_56.out	7.078302	89.04	197.03	250.03	30.7628	-9.5363	-13.0747	30.8445	-39.5852	70.02842
M4 (92.9, 54.3)	Sucrose_288.out	3.086089	95.80	50.76	17.53	0.5397	-22.2779	33.9597	-34.2273	21.6128	17.53407
	Sucrose_772.out	4.686865	94.68	43.96	12.72	3.6655	-25.7308	36.3752	-34.7617	19.9069	12.72093
	Sucrose_655.out	4.983049	98.43	53.32	22.99	-2.7698	-19.1239	31.9053	-34.3539	23.6661	22.99251
	Sucrose_637.out	5.480036	98.64	53.31	20.19	-1.1252	-20.9477	33.1464	-34.5361	22.8013	20.1906
	Sucrose_919.out	9.339216	95.20	50.65	16.89	0.9181	-22.732	34.3748	-34.355	21.4223	16.89221
	Sucrose_1379.out	9.477268	93.98	53.77	17.17	0.7987	-22.7052	34.4643	-34.6079	21.667	17.16883
	Sucrose_479.out	9.661129	89.66	51.13	15.23	1.9873	-23.6987	34.8861	-34.2411	20.6674	15.22542
	Sucrose_1226.out	10.76241	93.90	48.95	18.78	-0.2429	-21.5337	33.3792	-34.2406	21.975	18.77623
	Sucrose_909.out	12.20317	87.01	47.54	14.30	2.642	-23.956	34.6122	-33.9231	19.836	14.3041

Table S9. Table showing selected conformers of 2-*epi* sucrose clusters, sorted based on their DFT energies, ΔG (M06-2X[8]/6-31+g(d,p)), glycosidic dihedral angles, φ and ψ, as well as the fructosyl pucker phase, P (derived from equation S2) .[6]

2-epi Sucrose										
Conformer	ΔG (Kcal/mol)	ϕ	Ψ	Pucker phase, P	Fructosyl dihedral angle					Cal. P
					A	B	C	D	E	
Sucrose_C_31.out	0	91.84	55.65	143.26	-32.2374	38.4605	-30.3669	12.9533	12.0162	-36.7386
Sucrose_C_60.out	0.270456	91.63	55.82	146.43	-30.1758	37.4886	-30.7801	14.5262	9.7372	-33.5731
Sucrose_C_36.out	0.312499	89.44	53.51	141.73	-33.1096	38.8103	-30.0257	12.1171	13.1059	-38.2725
Sucrose_C_75.out	0.518322	89.29	54.09	144.44	-31.2521	37.8934	-30.3349	13.4771	11.0794	-35.5625
Sucrose_C_35.out	1.570028	88.07	55.65	137.65	-34.3305	38.2963	-28.0866	9.4245	15.598	-42.3523
Sucrose_C_72.out	1.785891	91.57	57.37	152.17	-26.0298	35.1405	-30.7075	16.8882	5.6097	-27.8301
Sucrose_C_156.out	1.802206	91.38	57.64	153.71	-25.0796	34.6129	-30.7799	17.5079	4.6145	-26.2904
Sucrose_C_15.out	2.082702	97.28	50.02	167.17	-17.2446	30.0232	-31.0549	22.2382	-3.2689	-12.8263
Sucrose_C_41.out	2.139806	91.27	57.70	154.27	-24.7746	34.4776	-30.8522	17.7553	4.2631	-25.7304
Sucrose_C_54.out	2.307978	90.88	57.04	146.85	-28.4764	35.7003	-29.3229	14.1208	8.894	-33.1529
Sucrose_C_85.out	2.336216	91.53	57.52	152.44	-25.9463	35.1117	-30.8086	17.0327	5.4638	-27.5615
Sucrose_C_33.out	2.336216	98.85	49.11	163.01	-18.7072	29.817	-29.5844	19.8686	-0.8383	-16.9885
Sucrose_C_115.out	2.393319	91.68	57.53	151.36	-26.3603	35.157	-30.4464	16.4458	6.099	-28.6383
Sucrose_C_5.out	2.409635	89.02	65.54	55.05	-23.3828	-0.4373	21.9325	-36.0158	37.6331	55.0537
Sucrose_C_182.out	2.518194	89.47	55.42	148.84	-27.555	35.5111	-29.8469	15.1824	7.6535	-31.1567
Sucrose_C_74.out	2.535764	87.54	52.10	141.03	-33.5697	39.0474	-29.9112	11.7691	13.6187	-38.97
Sucrose_C_59.out	2.687621	89.67	55.44	149.04	-27.4822	35.5142	-29.9158	15.2909	7.5345	-30.9625
Sucrose_C_65.out	2.775472	90.48	49.76	138.89	-32.4324	36.7468	-27.3957	9.7947	14.1896	-41.1082
Sucrose_C_2.out	2.93737	88.92	66.00	53.95	-23.4181	-1.2567	23.2395	-37.4487	38.6599	53.95176
Sucrose_C_9.out	2.98004	85.85	61.88	58.20	-25.2421	1.712	20.3052	-35.4212	38.4201	58.20116
Sucrose_C_87.out	3.055969	87.41	52.45	141.05	-33.5797	39.067	-29.9351	11.7874	13.6132	-38.9498
Sucrose_C_131.out	3.363448	89.52	49.58	138.29	-32.7306	36.8211	-27.2265	9.4645	14.5844	-41.7051

Sucrose_C_369.out	3.408001	89.16	55.27	135.22	-36.9578	40.0162	-28.4594	8.1387	18.0805	-44.779
Sucrose_C_63.out	3.606922	93.71	49.62	146.18	-29.8516	37.1969	-30.324	14.2533	9.7243	-33.8178
Sucrose_C_61.out	3.675948	89.30	49.35	137.74	-33.0728	36.9633	-27.1276	9.17	14.9844	-42.255
Sucrose_C_58.out	3.746856	89.15	66.13	53.50	-23.2547	-1.5997	23.5638	-37.7064	38.6442	53.4994
Sucrose_C_37.out	3.947032	86.15	61.74	60.54	-27.1378	3.3434	19.4642	-35.7297	39.8301	60.53704
Sucrose_C_10.out	3.970249	89.03	64.56	54.17	-23.6776	-1.1358	23.2362	-37.6527	38.8601	54.17214
Sucrose_C_17.out	3.99033	88.94	64.90	55.01	-24.1607	-0.5429	22.7544	-37.4003	39.015	55.00503
Sucrose_C_29.out	3.99535	86.48	61.29	55.85	-24.6641	0.0626	22.295	-37.2317	39.2117	55.85356
Sucrose_C_106.out	4.148462	89.49	47.36	143.52	-31.3886	37.9597	-29.8783	12.9257	11.5623	-36.4763
Sucrose_C_262.out	4.225018	89.81	48.13	136.89	-33.2397	36.9296	-26.7165	8.679	15.478	-43.1088
Sucrose_C_4.out	4.228783	89.87	65.27	52.02	-22.5072	-2.6525	24.5208	-38.2943	38.5312	52.02488
Sucrose_C_134.out	6.681088	89.46	180.03	164.02	-16.3832	26.7729	-26.8074	18.2693	-1.2638	-15.9776
Sucrose_C_53.out	6.711836	100.42	214.20	36.48	-12.7902	-13.4744	32.4555	-40.5639	33.9663	36.47514
Sucrose_C_76.out	6.737564	95.67	182.41	157.74	-21.4547	31.5658	-29.3933	18.0555	2.0638	-22.2605
Sucrose_C_215.out	7.224511	92.94	184.47	169.34	-15.43	28.3954	-30.0495	22.1211	-4.2962	-10.6601
Sucrose_C_100.out	7.251494	103.52	193.92	90.42	-40.6804	24.0233	-0.3074	-22.8093	40.0848	-89.5752
Sucrose_C_252.out	7.255259	105.53	178.14	148.39	-27.857	35.7224	-29.8241	15.0722	7.9733	-31.6052
Sucrose_C_7.out	7.33056	106.56	190.76	42.09	-16.7543	-9.9491	30.3661	-40.9387	36.658	42.08542
Sucrose_C_150.out	7.332443	93.04	184.63	169.28	-15.4632	28.4187	-30.0512	22.1051	-4.2641	-10.7221
Sucrose_C_193.out	7.348758	91.68	194.02	11.57	3.511	-20.268	28.1694	-26.6813	14.8513	11.57296
Sucrose_C_148.out	7.475515	98.63	184.31	167.11	-16.9425	29.6745	-30.6388	21.8376	-3.1994	-12.8903
Sucrose_C_28.out	7.543913	99.91	211.66	34.54	-11.7897	-15.4702	34.2837	-42.0091	34.3036	34.54209
Sucrose_C_119.out	7.575289	90.40	194.10	11.20	3.8283	-21.06	29.1177	-27.483	15.1536	11.20248
Sucrose_C_49.out	7.99823	106.30	190.87	39.58	-14.9958	-11.43	31.1679	-40.3845	35.3406	39.57691
Sucrose_C_20.out	4.792914	112.61	189.64	137.95	-35.019	39.4874	-28.9229	9.9868	15.7757	-42.0516
Sucrose_C_84.out	5.729157	118.03	193.74	139.42	-33.8471	38.8206	-29.0058	10.7937	14.5962	-40.5837
Sucrose_C_99.out	5.949413	112.47	190.55	138.17	-34.8312	39.3819	-28.9583	10.0723	15.6362	-41.8323

Sucrose_C_79.out	6.230537	115.91	185.43	142.43	-31.0879	36.9116	-28.7464	11.9156	11.9756	-37.5702
Sucrose_C_431.out	7.29542	110.55	194.22	138.53	-33.7079	38.2651	-28.2787	10.0653	15.0097	-41.4694
Sucrose_C_273.out	7.633647	110.29	193.21	137.48	-34.5614	38.845	-28.2687	9.5286	15.902	-42.5204
Sucrose_C_218.out	6.998608	102.55	312.98	5.39	6.6546	-22.6081	28.9032	-25.5411	12.1077	5.385563
Sucrose_C_98.out	7.508145	112.57	309.42	339.21	25.8976	-39.7912	37.6121	-23.3006	-1.5603	-20.7897
Sucrose_C_210.out	7.753501	108.21	309.58	18.37	0.0171	-22.4735	34.8731	-35.5471	22.5787	18.36722
Sucrose_C_293.out	7.901593	104.63	312.46	10.37	3.913	-19.7323	27.0375	-25.2384	13.6326	10.36888
Sucrose_C_502.out	6.757644	89.42	314.43	18.26	0.0028	-17.6494	27.3003	-27.6948	17.687	18.26439
Sucrose_C_579.out	6.994215	96.24	314.87	13.01	2.7429	-20.4371	29.0384	-27.768	16.0658	13.01271
Sucrose_C_120.out	7.599761	77.29	312.06	32.50	-9.5199	-15.4789	32.2575	-38.5239	30.6708	32.49524
Sucrose_C_228.out	7.826292	94.33	315.25	23.24	-3.2202	-20.4732	34.1958	-36.8246	25.6226	23.23983
Sucrose_C_34.out	7.279732	75.87	53.67	343.13	21.7979	-35.6104	35.346	-23.3509	1.0756	-16.8666
Sucrose_C_11.out	7.51693	77.55	53.13	340.58	23.4699	-36.5893	35.2862	-22.4256	-0.6541	-19.4205
Sucrose_C_8.out	7.515048	120.05	76.78	341.66	23.2285	-36.8822	36.2251	-23.1958	-0.0414	-18.3392

Table S10. RDC and RCSA values of sucrose acquired in the $CDCl_3$/DMSO (70:30) PBLG LC solution.

Atom	Number of protons	RDC (Hz)	RCSA (Hz)
C8	-	-	-1.62
C5	1	52.25	-2.97
C11	1	-17.74	-1.55
C9	1	-19.79	1.23
C10	1	3.12	-2.24
C1	1	22.23	2.01
C3	1	23.32	-3.05
C4	1	21.30	-2.23
C2	1	17.53	2.83
C13	2	6.06	-3.59
C22	2	24.05	-4.23
C18	2	9.02	-1.27

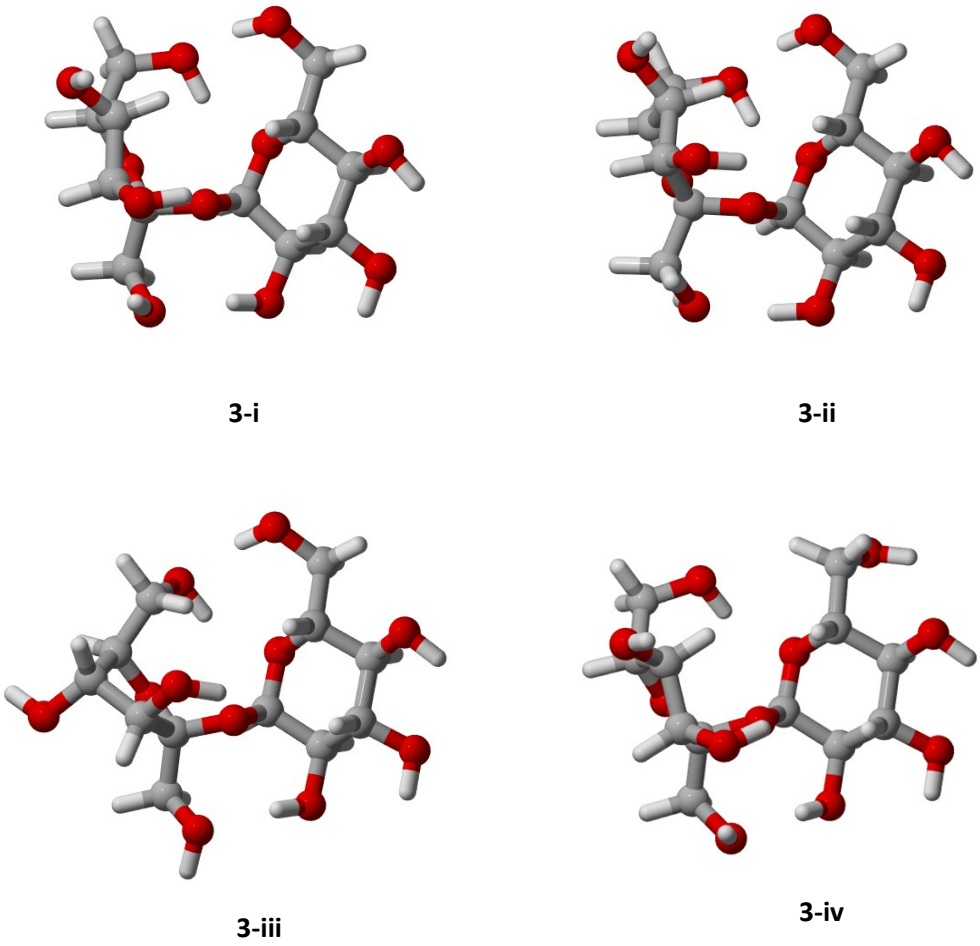

Figure S8. M1 cluster lowest energy conformers of sucrose, **3**, utilized for SVD analysis of RDC and RCSA data acquired in $CDCl_3$/DMSO-d_6 co-solvent mixture.

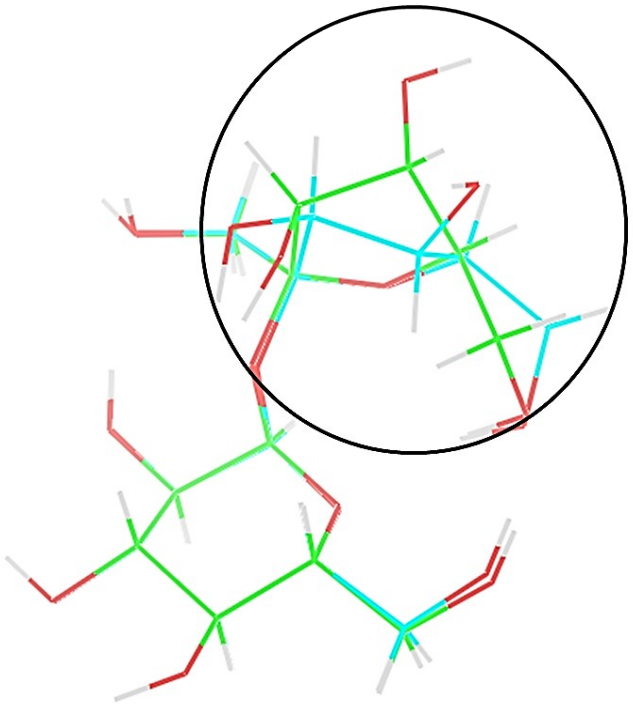

Figure S9. Global alignment of sucrose conformers, **3-i** and **3-iii**, reveal that both structures only vary with the fructosyl ring puckering – ignoring minor rotations of hydroxyl groups (heavy atoms at positions of variation are differentiated, **3-i** (cyan) and **3-iii** (green)).

Table S11. Table showing Q-factors of sucrose and 2-*epi* sucrose utilizing RDC and RCSA data measured in 70:30 $CDCl_3$/DMSO. $CDCl_3$ RQC is shown as well.

Q-values				
		RDC (Hz)	RCSA[a] (Hz)	RDC/RCSA (Hz)
Sucrose	M1	0.052	0.234	0.061
	M2	0.217	0.546	0.245
	M3	0.358	0.486	0.371
	M4	0.381	0.682	0.396
2-epi Sucrose		0.279	0.334	0.320
RQC		127.2		

[a]: SVD analysis with sucrose RCSA data alone gives significantly higher *Q*-values in all cases than that with sucrose RDC data alone, although it still provides clear differentiation of different conformational states and diastereomers. This is because sucrose has only sp^3-hybrized carbons which have small RCSAs, i.e. -4.2—2.8 Hz (Table S10). In comparison, RDC has a 10-fold larger data range of -19.8 — 52.3 Hz, and accordingly much lower Q-factors.

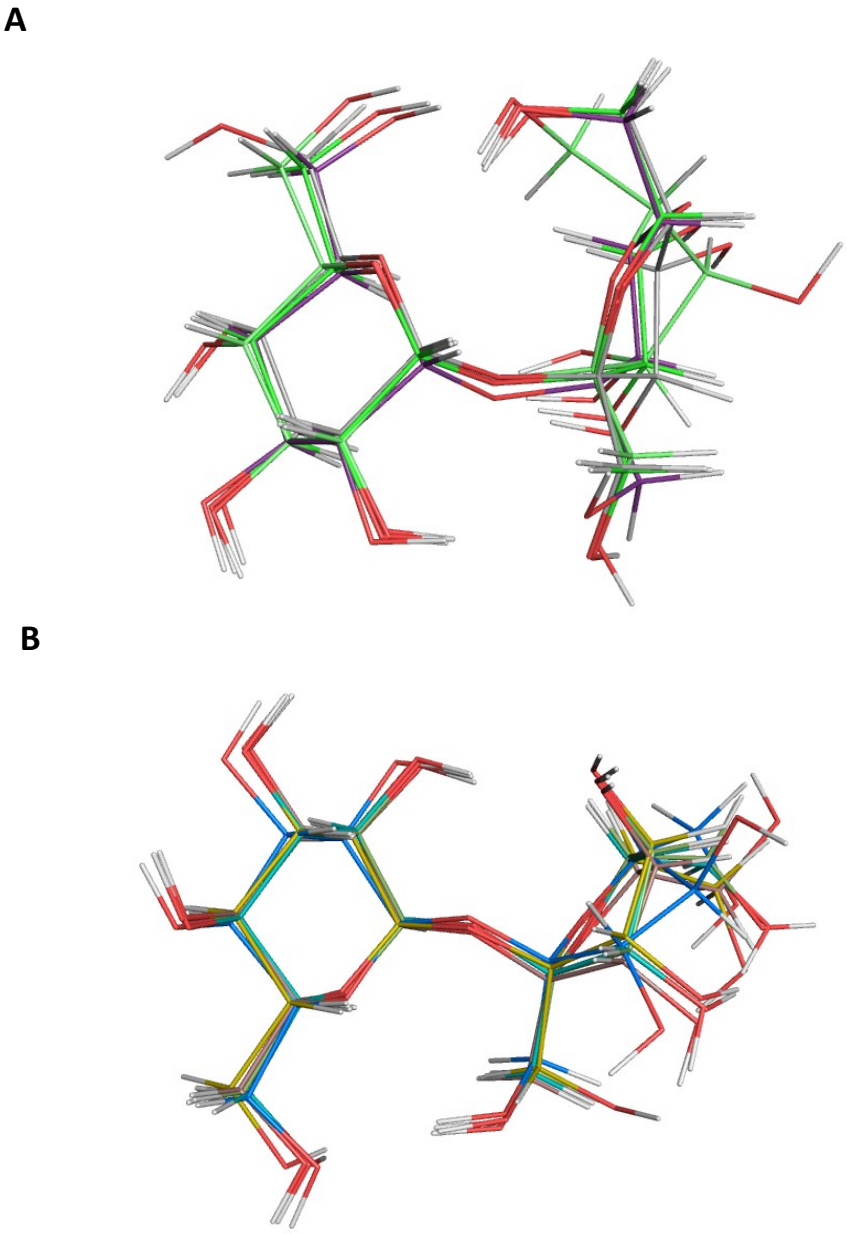

Figure S10. Heavy-atom superposition of (A) four M1 low energy conformers of sucrose and (B) five low energy conformers of 2′-*epi* sucrose.

Structure Coordinates and Chemical Shielding Tensors of Strychnine from DFT

Refer to supporting information of Ref 12

Structural Coordinates of Parthenolide from DFT

Table S12. Coordinates of parthenolide *E*-isomers.

Parthenolide DFT coordinates									
Atom	RRRRE			RRRSE			RRSRE		
C1	-3.038	-0.473	1.124	3.212	-0.301	-0.987	-3.467	0.136	0.484
C2	-2.632	-1.543	0.079	2.839	-1.257	0.171	-2.979	-1.07	-0.354
C3	-1.13	-1.725	-0.02	1.358	-1.593	0.184	-1.63	-1.568	0.12
C4	-0.457	-0.926	-1.052	0.513	-0.735	1.036	-0.446	-1.013	-0.561
C5	-1.944	1.658	0.221	1.863	1.73	-0.274	-1.689	1.852	-0.109
C6	-2.105	0.719	1.164	2.144	0.754	-1.144	-2.339	1.096	0.785
C7	0.93	-0.339	-1.009	-0.953	-0.413	0.966	0.878	-0.849	0.115
C8	1.034	0.863	-0.046	-1.397	1.014	0.544	1.27	0.555	0.644
C9	0.418	2.178	-0.545	-0.708	1.699	-0.664	0.866	1.793	-0.205
C10	-0.793	2.636	0.3	0.567	2.515	-0.382	-0.401	2.543	0.26
O11	1.932	-1.268	-0.556	-1.677	-1.31	0.096	1.921	-1.185	-0.843
C12	2.929	-0.599	0.067	-2.845	-0.74	-0.269	3.073	-0.581	-0.486
C13	2.507	0.824	0.261	-2.823	0.689	0.16	2.772	0.395	0.604
O14	-0.673	-2.314	-1.255	0.873	-2.049	1.46	-0.886	-2.346	-0.824
O15	3.958	-1.137	0.393	-3.707	-1.347	-0.855	4.129	-0.829	-1.014
C16	3.361	1.774	0.63	-3.912	1.454	0.151	3.724	0.965	1.337
C17	-0.438	-2.222	1.225	0.854	-2.354	-1.019	-1.589	-2.077	1.543

C18	-2.804	1.76	-1.01	2.756	2.1	0.88	-2.118	2.006	-1.544
H19	-3.055	-0.932	2.117	4.199	0.129	-0.786	-4.282	0.63	-0.057
H20	-4.068	-0.162	0.912	3.3	-0.868	-1.919	-3.893	-0.224	1.426
H21	-3.102	-2.5	0.337	3.086	-0.787	1.13	-2.884	-0.785	-1.407
H22	-2.999	-1.257	-0.913	3.419	-2.185	0.099	-3.712	-1.885	-0.297
H23	-1.108	-0.292	-1.658	1.038	0.048	1.587	-0.619	-0.331	-1.393
H24	-1.437	0.764	2.026	1.437	0.58	-1.954	-1.942	1.073	1.801
H25	1.216	-0.031	-2.024	-1.344	-0.585	1.979	0.969	-1.57	0.932
H26	0.518	0.551	0.874	-1.358	1.682	1.411	0.904	0.678	1.668
H27	0.115	2.069	-1.594	-1.453	2.397	-1.063	1.698	2.502	-0.138
H28	1.174	2.97	-0.53	-0.538	0.959	-1.455	0.791	1.52	-1.266
H29	-0.468	2.749	1.34	0.417	3.089	0.542	-0.343	2.68	1.346
H30	-1.111	3.623	-0.056	0.665	3.263	-1.18	-0.377	3.541	-0.195
H31	3.05	2.807	0.758	-3.882	2.491	0.473	3.488	1.666	2.133
H32	4.404	1.528	0.813	-4.864	1.047	-0.18	4.77	0.734	1.15
H33	0.616	-2.428	1.038	0.781	-1.697	-1.892	-1.684	-1.255	2.26
H34	-0.518	-1.485	2.032	1.56	-3.156	-1.259	-2.426	-2.764	1.706
H35	-0.921	-3.144	1.566	-0.126	-2.787	-0.829	-0.665	-2.62	1.75
H36	-3.585	0.997	-1.042	3.705	1.559	0.872	-3.064	1.505	-1.759
H37	-3.287	2.744	-1.048	2.976	3.175	0.853	-2.233	3.069	-1.786
H38	-2.205	1.674	-1.926	2.259	1.911	1.841	-1.361	1.611	-2.234
Atom	RRSSE			RSRRE			RSRSE		
C1	-3.326	-0.214	-0.87	-3.216	0.244	0.133	-3.309	-0.12	-0.186
C2	-2.688	-1.621	-0.806	-2.577	-0.921	-0.645	-2.405	-1.253	-0.708
C3	-1.526	-1.642	0.165	-1.616	-1.758	0.174	-1.383	-1.716	0.312

C4	-0.195	-1.352	-0.398	-0.161	-1.487	0.222	0.017	-1.228	0.327
C5	-1.88	1.775	-0.166	-1.47	2.078	-0.017	-1.717	1.862	-0.182
C6	-2.257	0.832	-1.04	-2.163	1.171	0.687	-2.465	0.951	0.452
C7	0.907	-0.651	0.345	0.533	-0.329	-0.451	0.629	-0.245	-0.647
C8	1.257	0.742	-0.245	1.162	0.646	0.579	1.226	1.041	-0.012
C9	0.592	1.975	0.401	1.058	2.133	0.187	0.457	1.751	1.105
C10	-0.604	2.557	-0.381	-0.281	2.773	0.598	-0.69	2.647	0.61
O11	2.105	-1.457	0.2	1.641	-0.865	-1.221	1.786	-0.911	-1.229
C12	3.194	-0.694	-0.001	2.818	-0.677	-0.596	2.914	-0.572	-0.575
C13	2.766	0.725	-0.165	2.591	0.171	0.609	2.603	0.551	0.358
O14	-0.554	-2.677	-0.018	-0.687	-2.508	-0.617	-0.316	-2.497	-0.233
O15	4.309	-1.156	-0.035	3.853	-1.139	-1.013	3.971	-1.119	-0.779
C16	3.657	1.711	-0.227	3.558	0.415	1.49	3.458	0.935	1.303
C17	-1.865	-1.365	1.61	-2.227	-2.524	1.323	-1.95	-2.257	1.603
C18	-2.609	2.13	1.105	-1.727	2.392	-1.468	-1.747	2.106	-1.667
H19	-4.03	-0.192	-1.71	-3.896	0.775	-0.54	-4.019	-0.519	0.547
H20	-3.909	-0.035	0.038	-3.832	-0.15	0.948	-3.904	0.269	-1.019
H21	-2.318	-1.911	-1.796	-3.363	-1.594	-1.011	-3.012	-2.124	-0.988
H22	-3.441	-2.358	-0.504	-2.053	-0.541	-1.528	-1.889	-0.922	-1.614
H23	-0.128	-1.225	-1.481	0.387	-1.875	1.086	0.555	-1.303	1.276
H24	-1.649	0.721	-1.942	-1.882	1.019	1.73	-2.343	0.877	1.535
H25	0.702	-0.581	1.417	-0.116	0.168	-1.172	-0.039	-0.039	-1.481
H26	0.991	0.718	-1.313	0.687	0.506	1.558	1.356	1.75	-0.845
H27	0.293	1.733	1.429	1.867	2.677	0.685	1.166	2.378	1.657
H28	1.35	2.76	0.486	1.229	2.236	-0.893	0.07	1.012	1.818
H29	-0.347	2.587	-1.447	-0.264	3.831	0.305	-0.275	3.454	-0.006

H30	-0.752	3.594	-0.055		-0.357	2.735	1.691		-1.158	3.119	1.481
H31	3.367	2.751	-0.343		3.386	1.029	2.371		3.236	1.741	1.996
H32	4.717	1.482	-0.163		4.55	-0.003	1.342		4.418	0.434	1.395
H33	-2.164	-0.324	1.756		-2.592	-1.839	2.094		-2.68	-3.047	1.392
H34	-2.702	-2.004	1.913		-3.073	-3.124	0.97		-1.153	-2.675	2.223
H35	-1.019	-1.587	2.262		-1.488	-3.192	1.773		-2.456	-1.469	2.169
H36	-3.479	1.501	1.302		-2.593	1.865	-1.872		-2.42	1.429	-2.199
H37	-1.941	2.074	1.973		-1.89	3.468	-1.596		-2.068	3.135	-1.87
H38	-2.955	3.169	1.045		-0.856	2.132	-2.085		-0.744	2.007	-2.1

Atom	RSSRE			RSSSE		
C1	3.009	-0.397	-0.965	3.133	-0.012	0.003
C2	2.137	-1.669	-0.854	2.23	-0.833	0.948
C3	1.265	-1.774	0.404	1.358	-1.861	0.245
C4	-0.057	-1.11	0.502	0.107	-1.621	-0.517
C5	1.892	1.773	-0.245	1.646	1.988	-0.389
C6	2.163	0.831	-1.158	2.264	0.885	-0.836
C7	-0.698	-0.373	-0.665	-0.657	-0.362	-0.881
C8	-1.305	1.029	-0.409	-0.863	0.726	0.191
C9	-0.526	2.097	0.357	-0.851	2.155	-0.399
C10	0.692	2.674	-0.404	0.457	2.536	-1.136
O11	-1.857	-1.183	-1.011	-2	-0.814	-1.227
C12	-2.963	-0.7	-0.403	-2.894	-0.491	-0.271
C13	-2.636	0.636	0.179	-2.225	0.385	0.73
O14	1.076	-0.573	1.162	0.063	-2.099	0.824
O15	-4.009	-1.302	-0.394	-4.038	-0.875	-0.303

C16	-3.43	1.24	1.06		-2.82	0.763	1.859	
C17	1.52	-2.992	1.258		2.099	-3.135	-0.102	
C18	2.602	1.926	1.071		1.915	2.617	0.952	
H19	3.684	-0.54	-1.817		3.727	-0.681	-0.628	
H20	3.633	-0.316	-0.071		3.842	0.559	0.611	
H21	2.804	-2.538	-0.859		2.851	-1.386	1.665	
H22	1.515	-1.764	-1.753		1.608	-0.149	1.532	
H23	-0.794	-1.549	1.18		-0.119	-2.396	-1.253	
H24	1.598	0.859	-2.092		1.985	0.509	-1.82	
H25	-0.059	-0.38	-1.544		-0.244	0.039	-1.809	
H26	-1.515	1.429	-1.414		-0.111	0.639	0.974	
H27	-1.229	2.916	0.547		-1.699	2.27	-1.085	
H28	-0.222	1.708	1.336		-1.028	2.846	0.432	
H29	0.428	2.796	-1.462		0.443	2.131	-2.153	
H30	0.91	3.671	-0.002		0.498	3.628	-1.222	
H31	-3.179	2.201	1.499		-2.317	1.396	2.584	
H32	-4.362	0.769	1.362		-3.832	0.434	2.079	
H33	1.342	-3.905	0.681		2.931	-2.923	-0.782	
H34	2.563	-2.999	1.595		2.51	-3.582	0.809	
H35	0.868	-2.996	2.135		1.436	-3.861	-0.579	
H36	3.397	1.195	1.222		2.816	2.229	1.43	
H37	3.044	2.928	1.131		2.027	3.702	0.841	
H38	1.9	1.831	1.907		1.075	2.46	1.642	

Table S13. Coordinates of parthenolide *Z*-isomers.

Parthenolide DFT coordinates									
Atom	RRRRZ			RRRSZ			RRSRZ		
C1	-2.977	-0.69	0.955	-3.247	-0.412	-0.676	-2.407	-0.526	-1.673
C2	-2.394	-1.976	0.324	-2.643	-1.701	-0.088	-2.166	-1.851	-0.93
C3	-0.893	-1.871	0.145	-1.149	-1.633	0.223	-1.143	-1.781	0.2
C4	-0.415	-0.99	-0.936	-0.234	-1.384	-0.914	0.238	-1.377	-0.138
C5	-2.297	1.54	-0.143	-2.162	1.746	0.139	-2.211	1.57	-0.236
C6	-3.048	0.433	-0.045	-3.11	0.8	0.208	-2.926	0.589	-0.803
C7	0.843	-0.145	-0.892	1.171	-0.825	-0.928	1.245	-0.809	0.837
C8	0.99	0.786	0.334	1.359	0.714	-0.977	1.308	0.729	1.006
C9	0.2	2.095	0.341	0.337	1.492	-0.129	-0.026	1.477	1.027
C10	-1.251	1.975	0.858	-1.016	1.706	-0.842	-0.708	1.681	-0.345
O11	2.024	-0.975	-0.873	1.914	-1.257	0.232	2.559	-1.166	0.331
C12	3.036	-0.322	-0.262	2.908	-0.385	0.503	3.139	-0.117	-0.291
C13	2.492	0.914	0.377	2.73	0.818	-0.361	2.323	1.108	-0.036
O14	-0.344	-2.403	-1.072	-0.39	-2.695	-0.39	-0.086	-2.747	0.083
O15	4.168	-0.74	-0.267	3.756	-0.61	1.331	4.164	-0.228	-0.918
C16	3.29	1.875	0.836	3.664	1.758	-0.479	2.553	2.259	-0.662
C17	-0.067	-2.199	1.367	-0.804	-1.367	1.668	-1.716	-1.65	1.591
C18	-2.479	2.477	-1.312	-2.133	2.901	1.106	-2.866	2.627	0.616
H19	-3.989	-0.911	1.313	-2.803	-0.228	-1.659	-1.482	-0.229	-2.177
H20	-2.387	-0.413	1.836	-4.312	-0.599	-0.854	-3.138	-0.721	-2.466
H21	-2.628	-2.84	0.956	-3.178	-1.971	0.831	-3.113	-2.222	-0.519
H22	-2.856	-2.148	-0.655	-2.796	-2.516	-0.804	-1.811	-2.596	-1.649
H23	-1.179	-0.544	-1.568	-0.709	-1.246	-1.889	0.45	-1.14	-1.184

H24	-3.783	0.268	-0.837	-3.859	0.895	0.997	-4.001	0.575	-0.613
H25	0.893	0.456	-1.809	1.674	-1.269	-1.796	1.14	-1.316	1.796
H26	0.695	0.208	1.221	1.345	1.073	-2.011	1.787	0.883	1.983
H27	0.721	2.78	1.019	0.775	2.461	0.131	-0.697	0.921	1.694
H28	0.235	2.563	-0.65	0.189	0.958	0.818	0.134	2.448	1.508
H29	-1.253	1.324	1.739	-0.971	2.651	-1.399	-0.448	2.674	-0.734
H30	-1.55	2.972	1.211	-1.173	0.919	-1.582	-0.321	0.962	-1.069
H31	2.904	2.784	1.288	3.521	2.625	-1.119	1.953	3.143	-0.47
H32	4.368	1.76	0.764	4.6	1.672	0.067	3.36	2.334	-1.386
H33	1.001	-2.067	1.181	0.271	-1.308	1.832	-2.317	-2.539	1.808
H34	-0.363	-1.584	2.223	-1.278	-0.439	2.002	-0.942	-1.567	2.358
H35	-0.239	-3.247	1.632	-1.207	-2.185	2.275	-2.372	-0.776	1.65
H36	-3.352	2.204	-1.911	-2.997	2.886	1.777	-3.952	2.502	0.648
H37	-2.6	3.513	-0.974	-2.127	3.858	0.569	-2.489	2.598	1.646
H38	-1.604	2.461	-1.974	-1.225	2.877	1.721	-2.645	3.628	0.227

Atom	RRSSZ			RSRRZ			RSRSZ		
C1	-3.401	0.174	-0.177	-3.221	0.061	-0.608	-3.167	-0.031	-0.532
C2	-2.946	-1.248	-0.565	-2.323	-1.149	-0.934	-2.387	-1.334	-0.806
C3	-1.66	-1.638	0.132	-1.568	-1.719	0.248	-1.447	-1.777	0.301
C4	-0.402	-1.215	-0.52	-0.11	-1.542	0.42	-0.023	-1.38	0.37
C5	-1.56	1.964	-0.241	-1.634	1.983	0.034	-1.636	1.997	-0.216
C6	-2.589	1.295	-0.785	-2.657	1.152	0.282	-2.481	1.252	-0.946
C7	0.849	-0.851	0.221	0.77	-0.735	-0.494	0.64	-0.452	-0.61
C8	1.191	0.649	0.102	1.072	0.677	0.065	1.125	0.89	-0.001
C9	0.569	1.577	1.141	0.72	1.806	-0.914	0.401	1.459	1.228

C10	-0.969	1.641	1.116	-0.785	1.919	-1.214	-1.136	1.566	1.14
O11	1.969	-1.54	-0.394	2.039	-1.428	-0.602	1.839	-1.11	-1.1
C12	3.074	-0.767	-0.375	3.059	-0.709	-0.099	2.956	-0.583	-0.565
C13	2.695	0.599	0.094	2.544	0.609	0.369	2.583	0.608	0.251
O14	-0.82	-2.574	-0.556	-0.639	-2.754	-0.105	-0.404	-2.652	-0.144
O15	4.158	-1.182	-0.704	4.191	-1.129	-0.069	4.051	-1.05	-0.764
C16	3.603	1.505	0.447	3.343	1.513	0.931	3.457	1.211	1.054
C17	-1.781	-1.941	1.607	-2.398	-2.029	1.47	-2.111	-2.228	1.581
C18	-0.954	3.151	-0.95	-1.272	3.077	1.008	-1.16	3.344	-0.697
H19	-4.436	0.296	-0.514	-4.132	-0.31	-0.128	-4.108	-0.087	-1.087
H20	-3.428	0.264	0.914	-3.545	0.494	-1.563	-3.447	0.012	0.526
H21	-2.796	-1.313	-1.648	-1.623	-0.914	-1.737	-3.104	-2.155	-0.932
H22	-3.73	-1.966	-0.294	-2.964	-1.952	-1.319	-1.838	-1.258	-1.749
H23	-0.491	-0.716	-1.486	0.291	-1.63	1.434	0.466	-1.433	1.346
H24	-2.917	1.614	-1.776	-3.194	1.308	1.218	-2.754	1.629	-1.933
H25	0.819	-1.166	1.269	0.366	-0.702	-1.508	0.009	-0.296	-1.484
H26	0.868	0.963	-0.903	0.504	0.819	0.993	1.066	1.625	-0.814
H27	0.898	1.268	2.141	1.268	1.653	-1.851	0.824	2.456	1.398
H28	0.974	2.583	0.977	1.083	2.749	-0.488	0.662	0.865	2.112
H29	-1.376	0.699	1.491	-0.939	2.838	-1.797	-1.459	2.293	1.897
H30	-1.274	2.42	1.829	-1.104	1.09	-1.852	-1.582	0.608	1.415
H31	3.324	2.489	0.811	2.968	2.474	1.274	3.183	2.064	1.668
H32	4.661	1.268	0.375	4.4	1.3	1.061	4.481	0.851	1.106
H33	-0.815	-2.162	2.063	-1.796	-2.556	2.214	-2.823	-3.032	1.367
H34	-2.255	-1.126	2.161	-2.786	-1.11	1.921	-1.365	-2.603	2.286
H35	-2.413	-2.829	1.719	-3.248	-2.664	1.195	-2.658	-1.409	2.057

H36	-1.478	3.365	-1.884		-1.981	3.123	1.838		-1.508	3.555	-1.712
H37	-1.011	4.043	-0.313		-1.265	4.051	0.504		-1.545	4.131	-0.035
H38	0.107	3.001	-1.182		-0.269	2.935	1.429		-0.069	3.432	-0.682

Atom	RSSRZ			RSSSZ		
C1	3.014	0.063	-0.345	2.603	0.236	-1.103
C2	2.44	-1.312	-0.765	2.755	-1.198	-0.565
C3	1.441	-1.926	0.221	1.672	-1.858	0.276
C4	0.043	-1.454	0.322	0.225	-1.548	0.279
C5	1.484	2.129	-0.223	1.406	2.23	-0.021
C6	2.302	1.286	-0.874	2.348	1.276	-0.046
C7	-0.519	-0.39	-0.597	-0.515	-0.53	-0.579
C8	-1.134	0.86	0.074	-1.064	0.661	0.238
C9	-0.478	1.482	1.311	-1.064	1.981	-0.554
C10	1.013	1.91	1.194	0.331	2.393	-1.069
O11	-1.63	-1.009	-1.298	-1.676	-1.202	-1.127
C12	-2.806	-0.67	-0.726	-2.795	-0.877	-0.443
C13	-2.553	0.399	0.284	-2.466	0.203	0.531
O14	1.014	-1.063	1.281	1.079	-1.058	1.306
O15	-3.849	-1.185	-1.046	-3.855	-1.415	-0.655
C16	-3.473	0.762	1.175	-3.34	0.626	1.442
C17	1.757	-3.333	0.666	2.071	-3.242	0.741
C18	0.975	3.386	-0.886	1.304	3.185	1.142
H19	3.089	0.094	0.745	3.566	0.467	-1.579
H20	4.039	0.111	-0.73	1.869	0.277	-1.908
H21	3.274	-2.017	-0.844	2.96	-1.866	-1.41

H22	1.999	-1.255	-1.768		3.656	-1.225	0.063	
H23	-0.71	-2.148	0.704		-0.439	-2.351	0.611	
H24	2.526	1.522	-1.917		3.038	1.234	0.8	
H25	0.201	-0.109	-1.362		0.067	-0.216	-1.441	
H26	-1.163	1.616	-0.723		-0.471	0.781	1.148	
H27	-0.579	0.791	2.155		-1.751	1.9	-1.405	
H28	-1.087	2.36	1.555		-1.472	2.757	0.104	
H29	1.14	2.844	1.757		0.573	1.823	-1.969	
H30	1.627	1.152	1.676		0.28	3.444	-1.38	
H31	-3.278	1.523	1.925		-3.087	1.407	2.153	
H32	-4.453	0.293	1.164		-4.333	0.188	1.491	
H33	1.791	-4.004	-0.199		1.309	-3.659	1.405	
H34	2.736	-3.36	1.157		3.02	-3.198	1.285	
H35	1.002	-3.7	1.365		2.196	-3.914	-0.114	
H36	1.189	3.399	-1.958		1.346	4.226	0.799	
H37	-0.104	3.516	-0.746		0.348	3.064	1.668	
H38	1.453	4.264	-0.432		2.108	3.026	1.866	

Chemical Shielding Tensors of Parthenolide from DFT

RRSSE

1 C Isotropic = 163.9131 Anisotropy = 14.3548
XX= 168.4822 YX= 0.5261 ZX= 0.6147
XY= 1.3774 YY= 170.8297 ZY= -7.7920
XZ= 5.3621 YZ= -7.1495 ZZ= 152.4274
Eigenvalues: 149.2651 168.9913 173.4830
2 C Isotropic = 152.5105 Anisotropy = 26.0153
XX= 156.5573 YX= -5.8796 ZX= 14.8214
XY= -1.4118 YY= 141.2349 ZY= 1.8755
XZ= 8.3649 YZ= 3.6063 ZZ= 159.7392
Eigenvalues: 138.5955 149.0819 169.8540
3 C Isotropic = 132.2038 Anisotropy = 52.7002
XX= 98.7157 YX= -10.1763 ZX= 31.7318
XY= -13.0620 YY= 145.0528 ZY= 14.6405
XZ= 27.5766 YZ= 7.0849 ZZ= 152.8429
Eigenvalues: 82.0355 147.2387 167.3373
4 C Isotropic = 125.1389 Anisotropy = 58.3382
XX= 106.8146 YX= 2.4828 ZX= 30.2711
XY= -0.7410 YY= 121.7559 ZY= -0.2586
XZ= 31.1426 YZ= 10.2415 ZZ= 146.8462
Eigenvalues: 90.0931 121.2926 164.0311
5 C Isotropic = 59.8126 Anisotropy = 151.8257
XX= 34.7698 YX= -49.1505 ZX= 73.7673
XY= -53.7323 YY= 99.9257 ZY= -19.4990
XZ= 76.4890 YZ= -26.4982 ZZ= 44.7424
Eigenvalues: -39.4516 57.8597 161.0297
6 C Isotropic = 68.4404 Anisotropy = 117.9903
XX= 48.4424 YX= -46.3590 ZX= 65.5781
XY= -33.6821 YY= 112.6524 ZY= -5.3581
XZ= 62.1704 YZ= -9.7693 ZZ= 44.2264
Eigenvalues: -21.5718 79.7924 147.1006
7 C Isotropic = 107.7517 Anisotropy = 45.6883
XX= 120.9752 YX= -12.0279 ZX= -6.2741
XY= -22.2684 YY= 119.0977 ZY= 3.0944
XZ= -9.5734 YZ= 1.6730 ZZ= 83.1822
Eigenvalues: 81.5520 103.4925 138.2105
8 C Isotropic = 142.0598 Anisotropy = 8.0964
XX= 143.1097 YX= -5.8451 ZX= -2.3350
XY= -3.7777 YY= 142.0586 ZY= -0.3796
XZ= -3.7128 YZ= -5.1769 ZZ= 141.0113
Eigenvalues: 134.9721 143.7500 147.4574
9 C Isotropic = 155.8961 Anisotropy = 21.9915
XX= 161.0525 YX= -6.8294 ZX= -0.3663
XY= -7.4269 YY= 163.4368 ZY= 7.6994
XZ= 2.7937 YZ= 8.0162 ZZ= 143.1988
Eigenvalues: 139.8963 157.2348 170.5571
10 C Isotropic = 147.7669 Anisotropy = 16.2629
XX= 155.0551 YX= 2.6331 ZX= -7.4271
XY= 3.4552 YY= 142.5354 ZY= -5.3340
XZ= -4.5141 YZ= 3.1351 ZZ= 145.7102

Eigenvalues: 141.7791 142.9128 158.6088
11 O Isotropic = 114.1168 Anisotropy = 152.9901
XX= 38.2026 YX= 157.3292 ZX= 7.0653
XY= 103.3265 YY= 112.8347 ZY= -3.4837
XZ= -15.6003 YZ= -18.0260 ZZ= 191.3132
Eigenvalues: -60.0837 186.3239 216.1102
12 C Isotropic = 32.3699 Anisotropy = 69.2096
XX= 58.4057 YX= -51.9866 ZX= 10.1570
XY= -37.0496 YY= -22.2692 ZY= 16.7162
XZ= 11.2290 YZ= 20.4346 ZZ= 60.9731
Eigenvalues: -46.2456 64.8456 78.5096
13 C Isotropic = 54.6526 Anisotropy = 125.0779
XX= 18.9515 YX= 50.4086 ZX= -11.2116
XY= 47.7628 YY= 10.1918 ZY= 14.0533
XZ= -10.6897 YZ= 25.8620 ZZ= 134.8145
Eigenvalues: -37.5518 63.4717 138.0379
14 O Isotropic = 261.1668 Anisotropy = 136.8517
XX= 315.0537 YX= 39.3779 ZX= 2.5562
XY= 46.9394 YY= 122.4238 ZY= 27.2301
XZ= 6.9965 YZ= 26.1903 ZZ= 346.0229
Eigenvalues: 110.5109 320.5882 352.4012
15 O Isotropic = -34.9590 Anisotropy = 561.5041
XX= -274.5258 YX= -1.8255 ZX= 58.7462
XY= 13.7007 YY= -151.4299 ZY= 72.5590
XZ= 82.4861 YZ= 67.4064 ZZ= 321.0786
Eigenvalues: -282.8240 -161.4300 339.3770
16 C Isotropic = 74.2665 Anisotropy = 155.4701
XX= 14.7129 YX= 47.8411 ZX= -11.8834
XY= 48.7598 YY= 32.5631 ZY= 13.6086
XZ= -20.3369 YZ= 16.3969 ZZ= 175.5237
Eigenvalues: -27.8558 72.7421 177.9133
17 C Isotropic = 171.2829 Anisotropy = 27.2588
XX= 167.4676 YX= -2.6560 ZX= -4.8665
XY= -1.8104 YY= 157.7662 ZY= 3.8375
XZ= -0.8566 YZ= 3.2567 ZZ= 188.6149
Eigenvalues: 157.0097 167.3836 189.4554
18 C Isotropic = 171.5051 Anisotropy = 19.3263
XX= 168.6701 YX= -4.4960 ZX= -9.5051
XY= -7.6700 YY= 172.9585 ZY= 0.4576
XZ= -14.3150 YZ= -0.1889 ZZ= 172.8867
Eigenvalues: 157.2915 172.8345 184.3893
19 H Isotropic = 30.1425 Anisotropy = 10.1329
XX= 32.3720 YX= -0.2391 ZX= 5.7216
XY= -0.9488 YY= 27.8927 ZY= -0.7608
XZ= 5.1727 YZ= -0.3366 ZZ= 30.1627
Eigenvalues: 25.7081 27.8215 36.8977
20 H Isotropic = 29.9353 Anisotropy = 4.7223
XX= 31.6504 YX= -1.1242 ZX= -2.5746
XY= -0.2072 YY= 29.7242 ZY= 1.5033
XZ= -1.0784 YZ= 2.1248 ZZ= 28.4314
Eigenvalues: 26.8576 29.8649 33.0835
21 H Isotropic = 31.0320 Anisotropy = 7.8681
XX= 29.3314 YX= -0.2548 ZX= 1.5621
XY= -0.3534 YY= 29.2119 ZY= 3.5183
XZ= 1.6738 YZ= 2.7894 ZZ= 34.5528

Eigenvalues: 27.2598 29.5589 36.2774
22 H Isotropic = 30.3176 Anisotropy = 7.8835
XX= 31.5397 YX= 3.3367 ZX= 0.1781
XY= 3.7774 YY= 32.3747 ZY= -0.2365
XZ= 1.5481 YZ= 0.1499 ZZ= 27.0384
Eigenvalues: 26.7295 28.6501 35.5733
23 H Isotropic = 29.8072 Anisotropy = 4.8644
XX= 27.9408 YX= 2.4651 ZX= 2.4755
XY= 2.0138 YY= 28.6319 ZY= 0.0422
XZ= -0.9740 YZ= -1.8177 ZZ= 32.8491
Eigenvalues: 25.8324 30.5391 33.0502
24 H Isotropic = 26.7780 Anisotropy = 3.6068
XX= 26.2849 YX= 1.6928 ZX= 2.9136
XY= 1.3077 YY= 27.8587 ZY= -0.2690
XZ= 2.0091 YZ= -0.8752 ZZ= 26.1903
Eigenvalues: 23.3001 27.8513 29.1825
25 H Isotropic = 28.6356 Anisotropy = 4.3214
XX= 30.9226 YX= -0.3593 ZX= -1.2184
XY= -0.6964 YY= 26.4574 ZY= 0.3205
XZ= -1.3089 YZ= -0.2150 ZZ= 28.5269
Eigenvalues: 26.3909 27.9994 31.5165
26 H Isotropic = 29.7298 Anisotropy = 2.5186
XX= 30.4164 YX= 0.4188 ZX= -0.4171
XY= 0.5479 YY= 28.2466 ZY= 0.1175
XZ= 2.2833 YZ= -0.7794 ZZ= 30.5262
Eigenvalues: 28.0230 29.7575 31.4088
27 H Isotropic = 30.5323 Anisotropy = 4.1512
XX= 30.3519 YX= -0.7372 ZX= -0.6475
XY= -0.8380 YY= 29.0432 ZY= 1.0456
XZ= -1.8035 YZ= 1.3856 ZZ= 32.2018
Eigenvalues: 28.5366 29.7605 33.2998
28 H Isotropic = 30.2560 Anisotropy = 8.8601
XX= 34.0890 YX= 2.2506 ZX= 0.9515
XY= 2.5644 YY= 32.3964 ZY= 1.4270
XZ= 1.2893 YZ= 2.5896 ZZ= 24.2825
Eigenvalues: 23.7819 30.8234 36.1627
29 H Isotropic = 30.1547 Anisotropy = 5.5944
XX= 29.3199 YX= 0.1859 ZX= -0.3870
XY= 1.1966 YY= 29.3383 ZY= -3.7362
XZ= 0.1024 YZ= -2.2906 ZZ= 31.8059
Eigenvalues: 27.1984 29.3814 33.8843
30 H Isotropic = 30.0079 Anisotropy = 7.2749
XX= 29.5513 YX= -1.0171 ZX= -0.2781
XY= -0.6594 YY= 34.7251 ZY= 0.1493
XZ= -0.8604 YZ= -0.2238 ZZ= 25.7473
Eigenvalues: 25.6611 29.5048 34.8578
31 H Isotropic = 26.9576 Anisotropy = 7.4717
XX= 29.6668 YX= 4.9539 ZX= -1.0741
XY= 2.2807 YY= 25.9440 ZY= -0.2014
XZ= -0.5915 YZ= 0.4044 ZZ= 25.2619
Eigenvalues: 23.5720 25.3620 31.9387
32 H Isotropic = 25.8957 Anisotropy = 5.6514
XX= 26.8191 YX= 2.1051 ZX= -0.4745
XY= 3.9239 YY= 26.3610 ZY= 0.0490
XZ= -0.9058 YZ= -0.0498 ZZ= 24.5071

Eigenvalues: 23.3668 24.6571 29.6633
33 H Isotropic = 30.7987 Anisotropy = 8.2769
XX= 27.2650 YX= -2.9506 ZX= -0.3306
XY= -2.3836 YY= 35.2343 ZY= 0.4214
XZ= -2.1269 YZ= 1.5777 ZZ= 29.8968
Eigenvalues: 26.2303 29.8491 36.3167
34 H Isotropic = 30.9684 Anisotropy = 8.9381
XX= 31.3662 YX= 3.0781 ZX= -2.2743
XY= 2.8801 YY= 29.8232 ZY= -2.2780
XZ= -4.0744 YZ= -2.9749 ZZ= 31.7159
Eigenvalues: 27.5050 28.4731 36.9272
35 H Isotropic = 31.4512 Anisotropy = 7.9606
XX= 31.4929 YX= -0.2538 ZX= 2.0915
XY= -0.1308 YY= 27.4373 ZY= -1.3598
XZ= 2.4380 YZ= -2.1406 ZZ= 35.4235
Eigenvalues: 27.0509 30.5446 36.7583
36 H Isotropic = 30.2417 Anisotropy = 5.0080
XX= 31.7082 YX= 2.2466 ZX= -1.9297
XY= 1.3295 YY= 30.8895 ZY= 2.3250
XZ= -3.6351 YZ= 0.7137 ZZ= 28.1273
Eigenvalues: 25.6727 31.4720 33.5803
37 H Isotropic = 30.5949 Anisotropy = 4.4016
XX= 30.2640 YX= -0.3295 ZX= 0.6384
XY= -0.6436 YY= 28.2811 ZY= 0.2717
XZ= 0.9899 YZ= 1.3102 ZZ= 33.2397
Eigenvalues: 27.9892 30.2662 33.5293
38 H Isotropic = 30.8854 Anisotropy = 10.1967
XX= 29.9272 YX= -4.0074 ZX= -1.9609
XY= -3.5564 YY= 35.4907 ZY= 1.0549
XZ= -1.2450 YZ= 1.1365 ZZ= 27.2384
Eigenvalues: 26.4240 28.5490 37.6833

RRRRE

1 C Isotropic = 165.3179 Anisotropy = 14.4851
XX= 166.1119 YX= 5.0296 ZX= -10.0267
XY= 3.7306 YY= 172.0881 ZY= 5.5881
XZ= -8.0026 YZ= 8.1439 ZZ= 157.7537
Eigenvalues: 149.1100 171.8690 174.9746
2 C Isotropic = 151.8175 Anisotropy = 29.2458
XX= 170.6126 YX= -6.5682 ZX= 2.3643
XY= -2.9979 YY= 138.5336 ZY= -0.7379
XZ= -2.3855 YZ= 4.9826 ZZ= 146.3062
Eigenvalues: 137.3440 146.7937 171.3147
3 C Isotropic = 133.3751 Anisotropy = 57.9141
XX= 153.2083 YX= -24.0664 ZX= 30.7028
XY= -23.7677 YY= 126.1742 ZY= 27.4476
XZ= 25.9912 YZ= 22.0013 ZZ= 120.7428
Eigenvalues: 79.8468 148.2940 171.9845
4 C Isotropic = 130.2240 Anisotropy = 51.4554
XX= 157.5256 YX= -7.8031 ZX= 14.4862
XY= -21.8726 YY= 118.7490 ZY= 16.4513
XZ= 16.5812 YZ= 19.4068 ZZ= 114.3974
Eigenvalues: 91.5287 134.6157 164.5276
5 C Isotropic = 56.5463 Anisotropy = 157.7936

XX= 38.6548 YX= -68.0804 ZX= -70.3678
XY= -73.5310 YY= 78.5147 ZY= 8.8219
XZ= -75.3408 YZ= 13.4003 ZZ= 52.4693
Eigenvalues: -46.5959 54.4927 161.7420
6 C Isotropic = 67.9601 Anisotropy = 117.8176
XX= 52.3458 YX= -56.2627 ZX= -71.6192
XY= -43.4552 YY= 97.4055 ZY= -8.8189
XZ= -63.0296 YZ= 0.8971 ZZ= 54.1291
Eigenvalues: -26.6139 83.9890 146.5052
7 C Isotropic = 111.8641 Anisotropy = 51.0605
XX= 113.4576 YX= -19.5930 ZX= 11.6826
XY= -22.5039 YY= 126.1330 ZY= -10.5287
XZ= 16.2086 YZ= -4.1561 ZZ= 96.0017
Eigenvalues: 87.6852 102.0028 145.9044
8 C Isotropic = 144.9210 Anisotropy = 8.1120
XX= 144.8282 YX= -7.9387 ZX= 3.2566
XY= -4.0146 YY= 143.0634 ZY= 0.3426
XZ= 3.0409 YZ= 8.7603 ZZ= 146.8714
Eigenvalues: 135.2853 149.1486 150.3290
9 C Isotropic = 162.1216 Anisotropy = 19.9009
XX= 162.2153 YX= -7.0863 ZX= -1.3413
XY= -7.2590 YY= 171.0529 ZY= -4.3372
XZ= -5.1076 YZ= -5.2605 ZZ= 153.0968
Eigenvalues: 149.7026 161.2734 175.3889
10 C Isotropic = 149.6436 Anisotropy = 17.5546
XX= 153.5597 YX= 5.7593 ZX= 5.8425
XY= 8.6804 YY= 152.0894 ZY= 7.1963
XZ= 3.2761 YZ= -3.0868 ZZ= 143.2817
Eigenvalues: 141.4878 146.0962 161.3467
11 O Isotropic = 120.1411 Anisotropy = 146.1361
XX= 65.7785 YX= 154.0629 ZX= -48.0549
XY= 98.0114 YY= 89.6900 ZY= 23.6249
XZ= -24.5798 YZ= 55.7709 ZZ= 204.9547
Eigenvalues: -59.7182 202.5763 217.5651
12 C Isotropic = 31.9474 Anisotropy = 72.4336
XX= 64.1272 YX= -45.9671 ZX= -17.0259
XY= -30.5575 YY= -11.2432 ZY= -35.2231
XZ= -19.4957 YZ= -45.2120 ZZ= 42.9583
Eigenvalues: -48.5632 64.1690 80.2365
13 C Isotropic = 54.6376 Anisotropy = 128.3410
XX= 21.0244 YX= 57.6413 ZX= -15.4218
XY= 49.2433 YY= 8.8122 ZY= -12.4662
XZ= -12.3481 YZ= -19.0743 ZZ= 134.0762
Eigenvalues: -38.9094 62.6239 140.1982
14 O Isotropic = 278.8539 Anisotropy = 129.2539
XX= 360.8019 YX= -1.2758 ZX= 8.5954
XY= 9.3442 YY= 167.8629 ZY= -98.9306
XZ= 13.4281 YZ= -70.3051 ZZ= 307.8970
Eigenvalues: 127.7515 343.7871 365.0232
15 O Isotropic = -44.4899 Anisotropy = 567.4112
XX= -174.9648 YX= 48.9639 ZX= -223.2924
XY= 71.6880 YY= -145.1235 ZY= -97.2596
XZ= -256.8896 YZ= -98.5788 ZZ= 186.6185
Eigenvalues: -295.5426 -171.7114 333.7842
16 C Isotropic = 77.1731 Anisotropy = 152.7192

XX= 21.8439 YX= 53.6719 ZX= -24.1374
XY= 50.8706 YY= 36.7312 ZY= -13.3164
XZ= -13.2685 YZ= -17.8966 ZZ= 172.9443
Eigenvalues: -23.5906 76.1240 178.9859
17 C Isotropic = 173.0067 Anisotropy = 26.6798
XX= 174.3275 YX= -5.5314 ZX= 7.0774
XY= -5.7056 YY= 166.5022 ZY= -11.1098
XZ= 12.0222 YZ= -7.5168 ZZ= 178.1903
Eigenvalues: 161.3395 166.8873 190.7932
18 C Isotropic = 171.9521 Anisotropy = 22.8088
XX= 173.6281 YX= -7.8243 ZX= 11.8385
XY= -7.2054 YY= 170.8490 ZY= -1.7914
XZ= 14.1486 YZ= 3.5683 ZZ= 171.3793
Eigenvalues: 156.9426 171.7557 187.1580
19 H Isotropic = 30.2074 Anisotropy = 7.9001
XX= 28.0479 YX= 1.2589 ZX= -3.5391
XY= 0.7062 YY= 28.7384 ZY= -1.6231
XZ= -2.0648 YZ= -1.5539 ZZ= 33.8358
Eigenvalues: 26.8465 28.3015 35.4741
20 H Isotropic = 29.8254 Anisotropy = 8.5410
XX= 34.9665 YX= -1.6808 ZX= -0.9307
XY= -1.2786 YY= 28.3083 ZY= 0.0052
XZ= -2.2634 YZ= -0.7286 ZZ= 26.2016
Eigenvalues: 25.7591 28.1977 35.5194
21 H Isotropic = 30.3741 Anisotropy = 7.6915
XX= 31.1941 YX= 3.8019 ZX= -1.4795
XY= 2.8808 YY= 32.8987 ZY= 0.0664
XZ= -0.2598 YZ= 0.6729 ZZ= 27.0295
Eigenvalues: 26.6043 29.0163 35.5018
22 H Isotropic = 30.9653 Anisotropy = 6.1419
XX= 32.6606 YX= -1.3751 ZX= 2.9630
XY= -0.6250 YY= 29.3607 ZY= 0.3302
XZ= 3.1507 YZ= -0.2605 ZZ= 30.8745
Eigenvalues: 28.2110 29.6249 35.0599
23 H Isotropic = 29.8029 Anisotropy = 7.8345
XX= 31.0540 YX= -3.5067 ZX= 3.7029
XY= -1.3165 YY= 32.1260 ZY= -1.3470
XZ= 1.2288 YZ= -2.1184 ZZ= 26.2287
Eigenvalues: 25.1161 29.2667 35.0259
24 H Isotropic = 26.5019 Anisotropy = 4.2898
XX= 24.6564 YX= 1.2638 ZX= -2.7584
XY= 1.0162 YY= 27.7931 ZY= -0.7160
XZ= -2.0592 YZ= -0.4714 ZZ= 27.0561
Eigenvalues: 23.0693 27.0746 29.3617
25 H Isotropic = 28.1385 Anisotropy = 4.2165
XX= 27.5633 YX= -1.0636 ZX= -1.7501
XY= -1.3626 YY= 26.4461 ZY= -2.0072
XZ= -0.1848 YZ= -0.7705 ZZ= 30.4061
Eigenvalues: 25.1271 28.3388 30.9495
26 H Isotropic = 29.3746 Anisotropy = 5.6792
XX= 31.5014 YX= 1.4152 ZX= -0.8051
XY= 1.3338 YY= 28.4666 ZY= -1.0144
XZ= -3.8550 YZ= -0.0907 ZZ= 28.1560
Eigenvalues: 26.9443 28.0189 33.1608
27 H Isotropic = 30.6556 Anisotropy = 5.0454

XX= 29.3492 YX= -0.7412 ZX= 0.3228
XY= -0.8702 YY= 29.4091 ZY= -1.2779
XZ= 1.5495 YZ= -1.7372 ZZ= 33.2084
Eigenvalues: 28.5247 29.4229 34.0192
28 H Isotropic = 30.3179 Anisotropy = 8.7410
XX= 33.0057 YX= 2.8749 ZX= -0.3618
XY= 3.1607 YY= 32.9833 ZY= -0.8097
XZ= -0.4471 YZ= -1.8224 ZZ= 24.9648
Eigenvalues: 24.7535 30.0551 36.1453
29 H Isotropic = 30.2223 Anisotropy = 6.8889
XX= 29.0586 YX= 0.8044 ZX= 0.4346
XY= 1.6324 YY= 29.5426 ZY= 4.2837
XZ= -0.3574 YZ= 3.1253 ZZ= 32.0657
Eigenvalues: 26.5126 29.3395 34.8149
30 H Isotropic = 30.0754 Anisotropy = 7.7354
XX= 29.5534 YX= -1.7637 ZX= 0.1718
XY= -1.6206 YY= 34.7243 ZY= -0.3764
XZ= 0.5187 YZ= 0.2054 ZZ= 25.9486
Eigenvalues: 25.9152 29.0788 35.2324
31 H Isotropic = 26.9941 Anisotropy = 7.4283
XX= 29.0889 YX= 4.7814 ZX= 2.0127
XY= 2.1521 YY= 26.2167 ZY= 0.6586
XZ= 1.5178 YZ= 0.6758 ZZ= 25.6767
Eigenvalues: 23.7760 25.2601 31.9463
32 H Isotropic = 26.0409 Anisotropy = 5.7664
XX= 26.7494 YX= 2.1086 ZX= 0.9377
XY= 3.6698 YY= 26.2409 ZY= 0.9693
XZ= 1.8317 YZ= 0.5125 ZZ= 25.1324
Eigenvalues: 23.4753 24.7622 29.8852
33 H Isotropic = 30.7013 Anisotropy = 8.5484
XX= 36.0423 YX= -1.5711 ZX= -0.0878
XY= -1.4695 YY= 28.2075 ZY= -3.3353
XZ= 0.1125 YZ= -4.2615 ZZ= 27.8541
Eigenvalues: 24.1361 31.5676 36.4003
34 H Isotropic = 30.9815 Anisotropy = 5.1482
XX= 28.5450 YX= -0.7468 ZX= 1.7949
XY= -0.5347 YY= 30.3060 ZY= 0.2512
XZ= 0.0492 YZ= 1.6325 ZZ= 34.0935
Eigenvalues: 28.1027 30.4281 34.4136
35 H Isotropic = 30.9696 Anisotropy = 9.7939
XX= 28.7043 YX= 0.6932 ZX= 0.4721
XY= 1.8084 YY= 34.3676 ZY= -4.4677
XZ= -0.9711 YZ= -4.9707 ZZ= 29.8368
Eigenvalues: 26.7535 28.6564 37.4988
36 H Isotropic = 30.3597 Anisotropy = 4.9478
XX= 31.9531 YX= 2.1603 ZX= 1.8449
XY= 1.5572 YY= 31.1613 ZY= -2.5618
XZ= 3.3248 YZ= -1.2454 ZZ= 27.9647
Eigenvalues: 25.5389 31.8820 33.6582
37 H Isotropic = 30.8790 Anisotropy = 10.2879
XX= 31.3987 YX= -4.6707 ZX= 2.2869
XY= -3.9463 YY= 34.0378 ZY= -1.3884
XZ= 1.6368 YZ= -1.4799 ZZ= 27.2005
Eigenvalues: 26.4113 28.4880 37.7376
38 H Isotropic = 30.7329 Anisotropy = 4.1422

XX= 30.5758 YX= -0.6012 ZX= -0.2627
XY= -0.7582 YY= 28.2198 ZY= 0.0838
XZ= -0.7175 YZ= -0.7416 ZZ= 33.4030
Eigenvalues: 28.0008 30.7034 33.4944

RSSSE

1 C Isotropic = 164.0508 Anisotropy = 14.9625
XX= 166.8641 YX= 1.9954 ZX= -0.5712
XY= 0.8935 YY= 165.5917 ZY= -9.8112
XZ= -1.7630 YZ= -11.1777 ZZ= 159.6965
Eigenvalues: 151.7434 166.3832 174.0258
2 C Isotropic = 152.2330 Anisotropy = 16.1945
XX= 150.5939 YX= 10.3726 ZX= 0.7909
XY= -0.3071 YY= 160.6155 ZY= 0.8729
XZ= -0.3751 YZ= 4.1015 ZZ= 145.4896
Eigenvalues: 145.0044 148.6653 163.0294
3 C Isotropic = 131.8902 Anisotropy = 57.8202
XX= 103.0512 YX= 9.1825 ZX= -26.4833
XY= 15.2013 YY= 164.5878 ZY= 16.2262
XZ= -29.6285 YZ= 15.0862 ZZ= 128.0316
Eigenvalues: 80.6112 144.6224 170.4369
4 C Isotropic = 125.9072 Anisotropy = 61.4443
XX= 106.5726 YX= -4.2351 ZX= -18.3101
XY= -9.6726 YY= 162.9956 ZY= 4.4190
XZ= -12.6412 YZ= 17.9502 ZZ= 108.1535
Eigenvalues: 91.7595 119.0921 166.8701
5 C Isotropic = 57.4249 Anisotropy = 160.2744
XX= 78.9567 YX= 45.7094 ZX= -72.3560
XY= 48.7104 YY= 89.1961 ZY= -19.4558
XZ= -81.6280 YZ= -28.5894 ZZ= 4.1219
Eigenvalues: -44.2505 52.2507 164.2745
6 C Isotropic = 66.4983 Anisotropy = 121.9451
XX= 97.6009 YX= 26.1465 ZX= -69.3144
XY= 19.0385 YY= 100.8651 ZY= -23.9247
XZ= -58.0163 YZ= -17.2873 ZZ= 1.0289
Eigenvalues: -31.1482 82.8480 147.7950
7 C Isotropic = 113.1739 Anisotropy = 49.5999
XX= 138.5048 YX= 11.8071 ZX= 10.2258
XY= 11.3166 YY= 109.6516 ZY= 9.5099
XZ= 14.3877 YZ= 5.9151 ZZ= 91.3654
Eigenvalues: 87.1855 106.0957 146.2406
8 C Isotropic = 152.0515 Anisotropy = 21.3944
XX= 160.6926 YX= -1.9424 ZX= -9.9904
XY= 1.8530 YY= 151.3594 ZY= 5.9574
XZ= -10.7757 YZ= 7.3527 ZZ= 144.1027
Eigenvalues: 136.6321 153.2081 166.3145
9 C Isotropic = 155.3803 Anisotropy = 29.3509
XX= 155.6862 YX= 0.8322 ZX= -12.7764
XY= 3.0125 YY= 166.2615 ZY= -9.2850
XZ= -18.5732 YZ= -12.3151 ZZ= 144.1931
Eigenvalues: 131.4297 159.7636 174.9475
10 C Isotropic = 153.9056 Anisotropy = 27.9304
XX= 161.1714 YX= -7.8071 ZX= 15.4587
XY= -5.5344 YY= 148.4423 ZY= -6.0230

XZ= 9.5340 YZ= -2.4878 ZZ= 152.1032
Eigenvalues: 143.3014 145.8896 172.5259
 11 O Isotropic = 112.4829 Anisotropy = 157.6578
XX= 6.8974 YX= -111.0031 ZX= -80.3635
XY= -81.5107 YY= 161.2679 ZY= -10.5551
XZ= -36.3592 YZ= -2.9359 ZZ= 169.2834
Eigenvalues: -53.2461 173.1067 217.5881
 12 C Isotropic = 32.0237 Anisotropy = 70.4344
XX= 69.5590 YX= 21.8419 ZX= 29.5907
XY= 15.7472 YY= 41.3222 ZY= -44.9243
XZ= 14.5832 YZ= -48.4410 ZZ= -14.8100
Eigenvalues: -48.1205 65.2117 78.9800
 13 C Isotropic = 54.4670 Anisotropy = 132.6111
XX= 16.5166 YX= -69.4911 ZX= -21.5706
XY= -70.2877 YY= 87.8705 ZY= -43.6267
XZ= -12.4081 YZ= -48.2034 ZZ= 59.0139
Eigenvalues: -41.7733 62.2999 142.8744
 14 O Isotropic = 272.5660 Anisotropy = 138.3542
XX= 291.1818 YX= -32.8411 ZX= 61.4965
XY= -47.8405 YY= 334.0493 ZY= 80.3946
XZ= 70.2922 YZ= 54.4386 ZZ= 192.4668
Eigenvalues: 129.4679 323.4279 364.8021
 15 O Isotropic = -34.4154 Anisotropy = 566.6351
XX= -242.5572 YX= -110.5797 ZX= 107.4954
XY= -100.2442 YY= 168.4538 ZY= -217.5501
XZ= 91.3117 YZ= -217.6337 ZZ= -29.1429
Eigenvalues: -283.0201 -163.5675 343.3413
 16 C Isotropic = 74.4461 Anisotropy = 149.7503
XX= 23.0175 YX= -71.5487 ZX= -3.3410
XY= -79.1302 YY= 111.7966 ZY= -46.3259
XZ= -2.0389 YZ= -48.8554 ZZ= 88.5242
Eigenvalues: -26.3839 75.4426 174.2797
 17 C Isotropic = 164.9513 Anisotropy = 40.5905
XX= 164.1125 YX= -14.4427 ZX= 2.9550
XY= -13.9088 YY= 182.5268 ZY= 12.5751
XZ= 8.7609 YZ= 13.0897 ZZ= 148.2147
Eigenvalues: 139.3546 163.4877 192.0117
 18 C Isotropic = 173.6377 Anisotropy = 23.6064
XX= 165.7983 YX= 10.8777 ZX= 4.3081
XY= 10.8131 YY= 175.2877 ZY= 7.5505
XZ= 7.8947 YZ= 3.8667 ZZ= 179.8270
Eigenvalues: 158.4937 173.0441 189.3752
 19 H Isotropic = 30.2886 Anisotropy = 7.3757
XX= 32.3130 YX= -2.5095 ZX= -3.7073
XY= -1.4281 YY= 29.9145 ZY= 1.1129
XZ= -2.9108 YZ= 1.0140 ZZ= 28.6382
Eigenvalues: 26.6880 28.9720 35.2057
 20 H Isotropic = 29.8819 Anisotropy = 7.7745
XX= 33.1804 YX= 2.3522 ZX= 3.0809
XY= 1.8580 YY= 30.1418 ZY= 0.8006
XZ= 1.7736 YZ= 1.3764 ZZ= 26.3234
Eigenvalues: 25.5112 29.0695 35.0648
 21 H Isotropic = 30.3385 Anisotropy = 6.6723
XX= 29.0296 YX= -0.3951 ZX= 3.0947
XY= -0.4050 YY= 30.6798 ZY= -1.9083

XZ= 3.7369 YZ= -2.4876 ZZ= 31.3062
Eigenvalues: 26.3251 29.9038 34.7867
22 H Isotropic = 30.6463 Anisotropy = 5.4926
XX= 29.5586 YX= -0.6674 ZX= -0.4283
XY= -0.8898 YY= 33.1659 ZY= 2.0828
XZ= -0.4535 YZ= 2.3007 ZZ= 29.2143
Eigenvalues: 28.2330 29.3978 34.3080
23 H Isotropic = 29.3430 Anisotropy = 9.1395
XX= 26.1182 YX= -3.1009 ZX= 2.5647
XY= -0.5585 YY= 32.0838 ZY= 6.3673
XZ= 3.5199 YZ= 2.2611 ZZ= 29.8271
Eigenvalues: 22.7689 29.8242 35.4360
24 H Isotropic = 26.4872 Anisotropy = 3.4789
XX= 27.2228 YX= -1.5747 ZX= -2.7559
XY= -1.3850 YY= 27.4077 ZY= -1.3255
XZ= -1.0085 YZ= -1.8575 ZZ= 24.8312
Eigenvalues: 22.8183 27.8369 28.8065
25 H Isotropic = 27.5437 Anisotropy = 3.6159
XX= 28.0125 YX= 2.0776 ZX= -0.2741
XY= 1.8693 YY= 27.6922 ZY= -1.3354
XZ= -0.1431 YZ= 0.0032 ZZ= 26.9265
Eigenvalues: 25.7598 26.9171 29.9543
26 H Isotropic = 29.6258 Anisotropy = 4.6918
XX= 31.8156 YX= -0.5286 ZX= 1.8931
XY= -1.5429 YY= 29.3389 ZY= -0.3370
XZ= 1.5088 YZ= -0.1122 ZZ= 27.7228
Eigenvalues: 27.0985 29.0252 32.7537
27 H Isotropic = 30.5310 Anisotropy = 6.6005
XX= 33.0384 YX= -1.5206 ZX= 2.9610
XY= -0.8844 YY= 30.2330 ZY= -3.0401
XZ= 1.3855 YZ= -2.2457 ZZ= 28.3216
Eigenvalues: 26.2667 30.3950 34.9313
28 H Isotropic = 30.4727 Anisotropy = 6.7963
XX= 29.6847 YX= -1.7564 ZX= -2.9607
XY= -0.2773 YY= 32.7526 ZY= 2.9721
XZ= -2.0059 YZ= 2.4034 ZZ= 28.9807
Eigenvalues: 26.4605 29.9540 35.0035
29 H Isotropic = 29.9696 Anisotropy = 5.5997
XX= 28.1395 YX= 0.4280 ZX= 0.1366
XY= 0.0130 YY= 28.2349 ZY= -1.6774
XZ= -0.9321 YZ= -0.0388 ZZ= 33.5344
Eigenvalues: 27.9477 28.2584 33.7027
30 H Isotropic = 30.1254 Anisotropy = 8.3269
XX= 27.8348 YX= 0.5593 ZX= -0.3507
XY= 0.8623 YY= 34.4640 ZY= -2.4648
XZ= 0.0959 YZ= -3.4194 ZZ= 28.0774
Eigenvalues: 26.9063 27.7933 35.6767
31 H Isotropic = 26.9791 Anisotropy = 7.5504
XX= 26.7251 YX= -1.9702 ZX= -4.5047
XY= -0.9938 YY= 24.9319 ZY= -0.0816
XZ= -2.6178 YZ= 1.0690 ZZ= 29.2802
Eigenvalues: 23.5162 25.4083 32.0127
32 H Isotropic = 26.0674 Anisotropy = 6.0003
XX= 25.9690 YX= -0.8125 ZX= -1.8165
XY= -2.3510 YY= 24.4510 ZY= 1.2316

XZ= -3.3147 YZ= 0.4766 ZZ= 27.7822
Eigenvalues: 23.2966 24.8381 30.0676
33 H Isotropic = 30.6179 Anisotropy = 8.1504
XX= 32.1931 YX= -0.9768 ZX= -4.0867
XY= -2.8387 YY= 30.8421 ZY= 2.2515
XZ= -3.6572 YZ= 1.4777 ZZ= 28.8186
Eigenvalues: 26.2131 29.5892 36.0516
34 H Isotropic = 30.9505 Anisotropy = 9.1797
XX= 29.5367 YX= -2.8399 ZX= 2.9864
XY= -3.9424 YY= 33.3580 ZY= -3.3122
XZ= 1.8013 YZ= -1.9854 ZZ= 29.9568
Eigenvalues: 27.1496 28.6316 37.0703
35 H Isotropic = 31.5978 Anisotropy = 10.0517
XX= 29.6148 YX= -0.1339 ZX= 1.3080
XY= 0.4328 YY= 36.5933 ZY= 4.1314
XZ= 2.1912 YZ= 3.7940 ZZ= 28.5852
Eigenvalues: 26.2251 30.2693 38.2989
36 H Isotropic = 30.3021 Anisotropy = 5.8618
XX= 31.4897 YX= -1.7299 ZX= 3.1417
XY= -0.6992 YY= 30.5501 ZY= 2.6041
XZ= 4.4829 YZ= 0.8856 ZZ= 28.8666
Eigenvalues: 25.2878 31.4086 34.2100
37 H Isotropic = 30.8824 Anisotropy = 9.8940
XX= 28.1723 YX= 3.0167 ZX= 1.7557
XY= 1.7838 YY= 36.6412 ZY= 0.9357
XZ= 1.2119 YZ= 1.1638 ZZ= 27.8335
Eigenvalues: 26.4285 28.7403 37.4784
38 H Isotropic = 30.6515 Anisotropy = 4.7196
XX= 31.4325 YX= 0.7888 ZX= -1.8651
XY= 1.2406 YY= 28.3168 ZY= 1.1633
XZ= -1.9416 YZ= 1.5810 ZZ= 32.2051
Eigenvalues: 27.2486 30.9079 33.7979

RSSRE

1 C Isotropic = 159.2604 Anisotropy = 16.1314
XX= 164.2196 YX= 0.7257 ZX= -6.4152
XY= 0.1877 YY= 166.4231 ZY= -6.7256
XZ= -9.3244 YZ= -5.2003 ZZ= 147.1385
Eigenvalues: 142.8208 164.9457 170.0146
2 C Isotropic = 157.3980 Anisotropy = 26.3671
XX= 153.6956 YX= 7.8599 ZX= -13.7565
XY= 2.3526 YY= 158.5668 ZY= -4.7391
XZ= -16.0315 YZ= -4.8652 ZZ= 159.9315
Eigenvalues: 141.5400 155.6778 174.9761
3 C Isotropic = 125.9301 Anisotropy = 69.8225
XX= 84.6638 YX= 30.9164 ZX= -5.5522
XY= 27.6460 YY= 134.0732 ZY= -18.0076
XZ= -10.3652 YZ= -14.8348 ZZ= 159.0535
Eigenvalues: 71.0567 134.2553 172.4785
4 C Isotropic = 125.7381 Anisotropy = 58.1584
XX= 100.2358 YX= 25.7414 ZX= 4.9181
XY= 14.0784 YY= 131.1807 ZY= -27.8738
XZ= 5.7256 YZ= -19.9792 ZZ= 145.7978
Eigenvalues: 86.0807 126.6233 164.5104

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  5  C    Isotropic =    37.1377   Anisotropy =   181.0478
XX=    27.4059   YX=    76.3746   ZX=   -75.8625
XY=    85.4630   YY=    66.0824   ZY=    -5.6985
XZ=   -85.4653   YZ=   -16.5367   ZZ=    17.9248
Eigenvalues:   -77.0896    30.6664   157.8362
  6  C    Isotropic =    56.1192   Anisotropy =   124.9968
XX=    54.1851   YX=    63.6556   ZX=   -70.1919
XY=    47.8829   YY=    86.9983   ZY=     8.6010
XZ=   -64.7731   YZ=    18.3425   ZZ=    27.1743
Eigenvalues:   -45.0027    73.9100   139.4504
  7  C    Isotropic =   108.2719   Anisotropy =    60.3819
XX=   127.7885   YX=    20.0193   ZX=    15.4466
XY=    20.1054   YY=   112.0599   ZY=    11.6514
XZ=    21.7375   YZ=     8.9397   ZZ=    84.9672
Eigenvalues:    77.7517    98.5375   148.5265
  8  C    Isotropic =   134.7361   Anisotropy =    20.6368
XX=   145.5796   YX=    -0.0589   ZX=     6.3240
XY=     9.6423   YY=   135.5523   ZY=    -0.2386
XZ=     4.9876   YZ=    -1.2568   ZZ=   123.0765
Eigenvalues:   121.4818   134.2325   148.4940
  9  C    Isotropic =   159.9219   Anisotropy =    18.8244
XX=   166.2107   YX=     7.1522   ZX=    -1.8100
XY=    11.5720   YY=   157.9193   ZY=     1.7717
XZ=    -7.5436   YZ=     6.7833   ZZ=   155.6359
Eigenvalues:   147.2704   160.0239   172.4715
 10  C    Isotropic =   144.7205   Anisotropy =    22.6326
XX=   153.9525   YX=    -9.2563   ZX=     6.6073
XY=    -5.0428   YY=   141.5073   ZY=    -7.2679
XZ=     4.6926   YZ=    -3.4225   ZZ=   138.7016
Eigenvalues:   134.5773   139.7753   159.8089
 11  O    Isotropic =    88.0456   Anisotropy =   156.0169
XX=    34.2139   YX=  -152.6662   ZX=   -47.6973
XY=  -118.6303   YY=    64.9379   ZY=   -41.2354
XZ=    -3.4363   YZ=   -33.8075   ZZ=   164.9848
Eigenvalues:   -94.4359   166.5157   192.0568
 12  C    Isotropic =    13.1461   Anisotropy =    75.2314
XX=    27.5356   YX=    54.7099   ZX=    34.9777
XY=    43.2150   YY=   -11.1290   ZY=   -47.7026
XZ=    19.2573   YZ=   -50.6972   ZZ=    23.0318
Eigenvalues:   -76.0696    52.2076    63.3004
 13  C    Isotropic =    38.2998   Anisotropy =   150.8233
XX=    33.3658   YX=   -75.9082   ZX=    22.8122
XY=   -78.4153   YY=    -4.6976   ZY=   -41.9653
XZ=    32.7721   YZ=   -42.9970   ZZ=    86.2311
Eigenvalues:   -67.0536    43.1043   138.8486
 14  O    Isotropic =   267.4216   Anisotropy =   148.9991
XX=   306.3992   YX=   -64.9274   ZX=   -56.7578
XY=   -60.4890   YY=   237.6553   ZY=  -109.8122
XZ=   -34.4738   YZ=  -122.6187   ZZ=   258.2102
Eigenvalues:   102.1526   333.3578   366.7543
 15  O    Isotropic =   -66.1997   Anisotropy =   592.6498
XX=  -287.8922   YX=   -74.2748   ZX=   148.4629
XY=   -61.2375   YY=   -95.5186   ZY=  -201.6415
XZ=   109.6420   YZ=  -211.9203   ZZ=   184.8116
Eigenvalues:  -322.3395  -205.1598   328.9001
```

16 C Isotropic = 62.3612 Anisotropy = 173.3303
XX= 47.1369 YX= -80.3489 ZX= 36.0396
XY= -84.3549 YY= 20.2073 ZY= -45.6550
XZ= 45.6495 YZ= -41.5780 ZZ= 119.7392
Eigenvalues: -50.0831 59.2518 177.9147
17 C Isotropic = 160.4956 Anisotropy = 44.2383
XX= 142.7924 YX= -14.3963 ZX= -9.9920
XY= -7.3874 YY= 171.0752 ZY= -19.7790
XZ= -10.1927 YZ= -21.2897 ZZ= 167.6193
Eigenvalues: 130.6550 160.8440 189.9878
18 C Isotropic = 167.3242 Anisotropy = 24.6522
XX= 166.8558 YX= 8.1587 ZX= 11.5667
XY= 10.5366 YY= 164.9818 ZY= -0.6251
XZ= 15.4975 YZ= -2.0169 ZZ= 170.1349
Eigenvalues: 150.3623 167.8513 183.7590
19 H Isotropic = 29.7559 Anisotropy = 11.2739
XX= 31.9975 YX= -0.8548 ZX= -6.6154
XY= 0.1833 YY= 27.5804 ZY= -0.1938
XZ= -6.0163 YZ= 0.2474 ZZ= 29.6899
Eigenvalues: 24.4114 27.5846 37.2718
20 H Isotropic = 29.1285 Anisotropy = 5.5427
XX= 31.6439 YX= 0.8769 ZX= 2.8260
XY= 0.5816 YY= 28.7921 ZY= 1.3581
XZ= 1.1421 YZ= 2.2175 ZZ= 26.9496
Eigenvalues: 25.5437 29.0182 32.8237
21 H Isotropic = 30.1176 Anisotropy = 8.2918
XX= 28.7657 YX= -2.7791 ZX= -2.4062
XY= -3.3042 YY= 33.9034 ZY= -0.2017
XZ= -3.6547 YZ= 0.7671 ZZ= 27.6836
Eigenvalues: 24.7769 29.9304 35.6454
22 H Isotropic = 29.9545 Anisotropy = 6.2943
XX= 29.1067 YX= 0.1260 ZX= 0.6920
XY= 0.6515 YY= 27.5968 ZY= 2.4945
XZ= 0.9166 YZ= 2.1257 ZZ= 33.1599
Eigenvalues: 26.7588 28.9540 34.1507
23 H Isotropic = 29.6224 Anisotropy = 8.5552
XX= 32.4612 YX= 0.5081 ZX= -0.0550
XY= 3.2080 YY= 27.8559 ZY= -5.6683
XZ= -2.6445 YZ= -4.9849 ZZ= 28.5503
Eigenvalues: 22.8447 30.6967 35.3259
24 H Isotropic = 26.6610 Anisotropy = 3.7947
XX= 25.7915 YX= -0.7356 ZX= -3.9036
XY= -1.1824 YY= 28.1942 ZY= 0.1591
XZ= -2.2634 YZ= -0.8257 ZZ= 25.9972
Eigenvalues: 22.6552 28.1369 29.1908
25 H Isotropic = 26.8107 Anisotropy = 4.9972
XX= 29.9626 YX= 0.4181 ZX= -0.7100
XY= 0.3770 YY= 25.0094 ZY= 0.1416
XZ= -1.0004 YZ= 0.4274 ZZ= 25.4600
Eigenvalues: 24.7602 25.5297 30.1421
26 H Isotropic = 28.7378 Anisotropy = 5.9958
XX= 27.5711 YX= -1.2230 ZX= 3.2540
XY= 0.0214 YY= 28.1001 ZY= -2.2037
XZ= 0.3221 YZ= -2.7408 ZZ= 30.5421
Eigenvalues: 26.2934 27.1849 32.7350

27 H Isotropic = 29.9046 Anisotropy = 9.5738
XX= 32.3693 YX= -2.4862 ZX= -2.7865
XY= -2.0144 YY= 32.5589 ZY= 2.7904
XZ= -3.5672 YZ= 2.8856 ZZ= 24.7857
Eigenvalues: 23.2034 30.2233 36.2872
28 H Isotropic = 29.8876 Anisotropy = 3.5366
XX= 30.5751 YX= -0.2517 ZX= 0.7805
XY= -1.1219 YY= 28.0198 ZY= 0.0597
XZ= 1.9984 YZ= 0.5008 ZZ= 31.0680
Eigenvalues: 27.7143 29.7032 32.2454
29 H Isotropic = 29.6961 Anisotropy = 6.5941
XX= 27.9104 YX= 0.2844 ZX= 0.0427
XY= -0.6280 YY= 29.6441 ZY= -4.0988
XZ= -0.5591 YZ= -2.6444 ZZ= 31.5339
Eigenvalues: 26.9937 28.0025 34.0922
30 H Isotropic = 29.4139 Anisotropy = 8.5171
XX= 28.4223 YX= 1.5246 ZX= -0.0146
XY= 1.4560 YY= 34.7244 ZY= 1.1658
XZ= 0.7288 YZ= -0.1512 ZZ= 25.0949
Eigenvalues: 25.0436 28.1061 35.0920
31 H Isotropic = 26.1872 Anisotropy = 7.7617
XX= 28.8523 YX= -3.0040 ZX= -3.3818
XY= -1.3803 YY= 23.5984 ZY= -0.0056
XZ= -2.3963 YZ= 1.6674 ZZ= 26.1109
Eigenvalues: 22.7834 24.4166 31.3617
32 H Isotropic = 25.1976 Anisotropy = 5.3988
XX= 26.3925 YX= -1.4405 ZX= -1.2641
XY= -2.8539 YY= 23.8923 ZY= 1.8444
XZ= -1.5876 YZ= 1.2285 ZZ= 25.3081
Eigenvalues: 22.4705 24.3256 28.7968
33 H Isotropic = 30.3144 Anisotropy = 10.2086
XX= 26.5961 YX= 0.1156 ZX= -0.5125
XY= -0.0059 YY= 37.1020 ZY= 1.3470
XZ= 0.7692 YZ= -0.5097 ZZ= 27.2450
Eigenvalues: 26.5716 27.2514 37.1201
34 H Isotropic = 30.1511 Anisotropy = 8.8286
XX= 31.9315 YX= -1.6427 ZX= 2.1892
XY= -3.4692 YY= 29.7948 ZY= -2.8972
XZ= 3.7970 YZ= -3.1425 ZZ= 28.7270
Eigenvalues: 26.0715 28.3450 36.0368
35 H Isotropic = 31.3351 Anisotropy = 10.6092
XX= 29.2234 YX= -0.1184 ZX= -3.2870
XY= 0.0599 YY= 30.5170 ZY= -4.9331
XZ= -3.1427 YZ= -4.8469 ZZ= 34.2650
Eigenvalues: 25.9051 29.6924 38.4079
36 H Isotropic = 29.6231 Anisotropy = 5.2283
XX= 31.1936 YX= -2.4008 ZX= 2.1556
XY= -1.2896 YY= 30.3853 ZY= 2.8255
XZ= 3.6654 YZ= 0.4865 ZZ= 27.2905
Eigenvalues: 24.7578 31.0030 33.1086
37 H Isotropic = 30.6062 Anisotropy = 11.0470
XX= 30.4955 YX= 4.8685 ZX= 2.5853
XY= 4.1295 YY= 34.2961 ZY= 1.8966
XZ= 1.7042 YZ= 1.8426 ZZ= 27.0271
Eigenvalues: 25.9875 27.8603 37.9708

38 H Isotropic = 29.8286 Anisotropy = 3.7374
XX= 30.1326 YX= 0.8077 ZX= -1.0066
XY= 1.4265 YY= 27.4504 ZY= 0.0660
XZ= -0.9035 YZ= 0.8162 ZZ= 31.9028
Eigenvalues: 26.9324 30.2332 32.3202

RSRSE

1 C Isotropic = 161.5157 Anisotropy = 18.7524
XX= 165.6499 YX= -3.3987 ZX= 1.8243
XY= -3.0528 YY= 169.2458 ZY= 8.6540
XZ= 1.2615 YZ= 10.9702 ZZ= 149.6514
Eigenvalues: 145.2324 165.2973 174.0173
2 C Isotropic = 151.8193 Anisotropy = 22.1988
XX= 152.3322 YX= -14.8849 ZX= 11.2185
XY= -7.0603 YY= 151.6099 ZY= -1.3298
XZ= 6.4969 YZ= -0.9695 ZZ= 151.5158
Eigenvalues: 138.4099 150.4295 166.6185
3 C Isotropic = 123.1246 Anisotropy = 51.8539
XX= 84.1099 YX= -20.4723 ZX= -0.8577
XY= -25.0118 YY= 135.1479 ZY= -11.6765
XZ= 0.2348 YZ= -10.2017 ZZ= 150.1160
Eigenvalues: 75.2081 136.4717 157.6938
4 C Isotropic = 122.3897 Anisotropy = 49.8260
XX= 93.2319 YX= -16.8098 ZX= -7.4909
XY= -7.4537 YY= 128.8023 ZY= -12.5938
XZ= -7.9123 YZ= -20.9141 ZZ= 145.1349
Eigenvalues: 86.7030 124.8590 155.6070
5 C Isotropic = 40.4176 Anisotropy = 176.6073
XX= 82.7472 YX= -68.9551 ZX= -41.3435
XY= -69.9564 YY= 91.9530 ZY= -32.4975
XZ= -48.8113 YZ= -9.9552 ZZ= -53.4474
Eigenvalues: -77.9416 41.0386 158.1558
6 C Isotropic = 53.7801 Anisotropy = 148.8912
XX= 97.2941 YX= -56.7841 ZX= -50.4531
XY= -46.1636 YY= 100.2794 ZY= -13.2153
XZ= -51.3326 YZ= -26.0924 ZZ= -36.2331
Eigenvalues: -61.5420 69.8414 153.0410
7 C Isotropic = 104.9722 Anisotropy = 55.0188
XX= 122.1334 YX= -10.4375 ZX= -18.0067
XY= -16.0313 YY= 104.6429 ZY= 14.3501
XZ= -27.5029 YZ= 9.7992 ZZ= 88.1405
Eigenvalues: 75.7393 97.5260 141.6514
8 C Isotropic = 139.0964 Anisotropy = 19.8445
XX= 150.3782 YX= 1.0826 ZX= -4.5283
XY= -4.2781 YY= 141.2162 ZY= 3.2156
XZ= -8.3053 YZ= 0.9305 ZZ= 125.6948
Eigenvalues: 123.9701 140.9931 152.3261
9 C Isotropic = 154.0430 Anisotropy = 23.7486
XX= 166.3015 YX= -2.6382 ZX= 7.1431
XY= -10.2790 YY= 149.2647 ZY= -4.3591
XZ= 1.8651 YZ= -4.4739 ZZ= 146.5629
Eigenvalues: 143.2923 148.9613 169.8754
10 C Isotropic = 149.1299 Anisotropy = 19.3651
XX= 153.5789 YX= 9.0139 ZX= 2.2605

XY= 4.7862 YY= 148.9162 ZY= 0.5401
XZ= 12.8973 YZ= 4.7213 ZZ= 144.8945
Eigenvalues: 140.2545 145.0951 162.0400
 11 O Isotropic = 84.7402 Anisotropy = 166.2468
XX= 26.2989 YX= 136.0492 ZX= 91.9107
XY= 117.3212 YY= 100.6081 ZY= -53.0308
XZ= 46.8758 YZ= -55.7404 ZZ= 127.3136
Eigenvalues: -102.3929 161.0421 195.5714
 12 C Isotropic = 13.5219 Anisotropy = 74.6027
XX= 28.5728 YX= -44.3177 ZX= -46.2711
XY= -38.1373 YY= 12.9351 ZY= -50.2386
XZ= -29.7411 YZ= -51.0127 ZZ= -0.9420
Eigenvalues: -75.1420 52.4508 63.2571
 13 C Isotropic = 39.2246 Anisotropy = 146.9374
XX= 26.5039 YX= 73.1316 ZX= 1.3987
XY= 78.7734 YY= 28.9554 ZY= -64.2743
XZ= -4.5641 YZ= -63.2436 ZZ= 62.2144
Eigenvalues: -64.8683 45.3592 137.1828
 14 O Isotropic = 263.9761 Anisotropy = 148.0442
XX= 320.6647 YX= 38.4982 ZX= 6.7608
XY= 47.9188 YY= 154.8210 ZY= -106.0840
XZ= 9.0151 YZ= -81.1660 ZZ= 316.4426
Eigenvalues: 103.5887 325.6674 362.6722
 15 O Isotropic = -64.9441 Anisotropy = 590.1247
XX= -302.6999 YX= 86.6384 ZX= -96.8507
XY= 64.8632 YY= 36.6747 ZY= -251.1755
XZ= -69.2041 YZ= -256.7091 ZZ= 71.1930
Eigenvalues: -322.7244 -200.5803 328.4724
 16 C Isotropic = 62.2078 Anisotropy = 173.7768
XX= 37.2255 YX= 81.9882 ZX= -8.0579
XY= 88.0165 YY= 55.4698 ZY= -72.2165
XZ= -14.5842 YZ= -68.1612 ZZ= 93.9282
Eigenvalues: -50.9606 59.5250 178.0590
 17 C Isotropic = 164.6066 Anisotropy = 39.3280
XX= 160.8524 YX= 2.9183 ZX= -9.7904
XY= 7.7411 YY= 153.9873 ZY= -17.9169
XZ= -6.7589 YZ= -16.1884 ZZ= 178.9801
Eigenvalues: 145.2656 157.7290 190.8253
 18 C Isotropic = 165.4324 Anisotropy = 27.8277
XX= 158.4931 YX= -7.9476 ZX= 5.5846
XY= -5.2267 YY= 156.3109 ZY= -4.9653
XZ= 8.3047 YZ= 0.6655 ZZ= 181.4931
Eigenvalues: 150.4324 161.8806 183.9842
 19 H Isotropic = 29.7055 Anisotropy = 8.3436
XX= 33.3775 YX= 1.4315 ZX= -3.9512
XY= 0.6009 YY= 27.6214 ZY= -0.6770
XZ= -2.8743 YZ= -0.9545 ZZ= 28.1177
Eigenvalues: 26.3640 27.4846 35.2679
 20 H Isotropic = 29.2694 Anisotropy = 8.6488
XX= 32.1420 YX= -1.3304 ZX= 4.6403
XY= -1.6555 YY= 28.2885 ZY= -1.6637
XZ= 2.9082 YZ= -2.5258 ZZ= 27.3777
Eigenvalues: 24.8620 27.9109 35.0352
 21 H Isotropic = 29.9289 Anisotropy = 8.8290
XX= 29.5759 YX= 2.0814 ZX= 2.2590

XY= 2.5901 YY= 32.2419 ZY= 2.7926
XZ= 3.6016 YZ= 3.3701 ZZ= 27.9689
Eigenvalues: 25.4988 28.4730 35.8149
22 H Isotropic = 30.2703 Anisotropy = 4.6521
XX= 29.2637 YX= -0.4397 ZX= -0.0606
XY= -0.3064 YY= 28.7640 ZY= -1.0802
XZ= 0.1930 YZ= -2.1860 ZZ= 32.7833
Eigenvalues: 28.0911 29.3482 33.3717
23 H Isotropic = 29.4933 Anisotropy = 5.7208
XX= 27.6683 YX= 3.8442 ZX= 1.5339
XY= 2.8075 YY= 29.0586 ZY= -3.2604
XZ= 4.1989 YZ= -1.0634 ZZ= 31.7530
Eigenvalues: 23.4204 31.7523 33.3072
24 H Isotropic = 25.7891 Anisotropy = 5.9849
XX= 27.0307 YX= 1.9538 ZX= -3.1333
XY= 1.9122 YY= 28.3539 ZY= 0.2446
XZ= -1.3582 YZ= 1.6630 ZZ= 21.9829
Eigenvalues: 20.7853 26.8031 29.7791
25 H Isotropic = 27.6085 Anisotropy = 5.1896
XX= 30.1939 YX= -1.4181 ZX= 0.9249
XY= -1.9572 YY= 26.6433 ZY= -0.9901
XZ= 0.2546 YZ= -1.4087 ZZ= 25.9882
Eigenvalues: 24.9967 26.7605 31.0682
26 H Isotropic = 28.7894 Anisotropy = 5.4005
XX= 28.5835 YX= 1.4263 ZX= -1.5277
XY= -0.8669 YY= 29.2492 ZY= -3.2147
XZ= 0.6597 YZ= -3.6123 ZZ= 28.5355
Eigenvalues: 25.4543 28.5241 32.3897
27 H Isotropic = 29.7139 Anisotropy = 9.6453
XX= 32.4813 YX= 1.1058 ZX= 4.4127
XY= 0.3902 YY= 28.5527 ZY= 3.8328
XZ= 4.2241 YZ= 3.7647 ZZ= 28.1076
Eigenvalues: 23.5968 29.4007 36.1441
28 H Isotropic = 30.1511 Anisotropy = 3.7800
XX= 29.0017 YX= 0.2908 ZX= -0.9901
XY= 2.0286 YY= 30.2083 ZY= -0.9866
XZ= -1.9085 YZ= -0.7754 ZZ= 31.2432
Eigenvalues: 28.0441 29.7381 32.6710
29 H Isotropic = 30.1309 Anisotropy = 6.7499
XX= 28.0008 YX= 1.5288 ZX= 0.7824
XY= 1.2183 YY= 33.9450 ZY= -2.5293
XZ= 2.2291 YZ= -1.1567 ZZ= 28.4469
Eigenvalues: 26.0578 29.7041 34.6308
30 H Isotropic = 29.1791 Anisotropy = 9.0254
XX= 28.6033 YX= -2.6331 ZX= -1.6683
XY= -2.0494 YY= 30.3904 ZY= 5.1410
XZ= -1.3825 YZ= 3.7828 ZZ= 28.5437
Eigenvalues: 24.8803 27.4610 35.1961
31 H Isotropic = 26.2467 Anisotropy = 7.8485
XX= 29.2645 YX= 2.3649 ZX= 4.0248
XY= 0.7748 YY= 23.5013 ZY= -0.7657
XZ= 2.4511 YZ= 0.7743 ZZ= 25.9743
Eigenvalues: 22.7501 24.5110 31.4790
32 H Isotropic = 25.1244 Anisotropy = 5.4434
XX= 26.3705 YX= 1.1715 ZX= 1.5694

XY= 2.5366 YY= 23.3135 ZY= 1.1388
XZ= 2.3566 YZ= 0.6166 ZZ= 25.6892
Eigenvalues: 22.4383 24.1816 28.7534
33 H Isotropic = 30.4003 Anisotropy = 10.1797
XX= 30.6494 YX= 4.4031 ZX= -0.2888
XY= 5.3049 YY= 32.4851 ZY= -1.8423
XZ= -2.0340 YZ= -2.6891 ZZ= 28.0664
Eigenvalues: 26.3524 27.6618 37.1868
34 H Isotropic = 31.1573 Anisotropy = 10.0999
XX= 29.8263 YX= -0.8365 ZX= 1.9058
XY= -0.3449 YY= 29.5586 ZY= -5.1108
XZ= 2.0930 YZ= -5.0688 ZZ= 34.0869
Eigenvalues: 26.1461 29.4352 37.8906
35 H Isotropic = 30.1865 Anisotropy = 7.3649
XX= 28.7326 YX= -2.1430 ZX= -3.1154
XY= -0.7651 YY= 29.1874 ZY= -0.2160
XZ= -4.3163 YZ= 1.0492 ZZ= 32.6395
Eigenvalues: 26.1255 29.3376 35.0964
36 H Isotropic = 29.5617 Anisotropy = 5.7026
XX= 28.4595 YX= 2.6883 ZX= 2.1811
XY= 2.3197 YY= 29.1223 ZY= -1.4850
XZ= 4.0118 YZ= 0.2235 ZZ= 31.1034
Eigenvalues: 24.9574 30.3643 33.3634
37 H Isotropic = 30.0576 Anisotropy = 10.7396
XX= 27.4118 YX= -3.4492 ZX= 2.4670
XY= -2.5159 YY= 34.0210 ZY= -3.6367
XZ= 1.6189 YZ= -3.7068 ZZ= 28.7399
Eigenvalues: 25.9056 27.0498 37.2173
38 H Isotropic = 30.2486 Anisotropy = 4.2708
XX= 31.9205 YX= -0.9810 ZX= -1.2924
XY= -1.6147 YY= 27.7771 ZY= -1.0210
XZ= -1.7867 YZ= -1.6841 ZZ= 31.0481
Eigenvalues: 26.6860 30.9639 33.0958

RRSRE

1 C Isotropic = 161.8000 Anisotropy = 17.5249
XX= 167.1221 YX= 2.7922 ZX= -4.2504
XY= 1.7615 YY= 169.7302 ZY= 8.5149
XZ= -1.2112 YZ= 10.1515 ZZ= 148.5477
Eigenvalues: 144.5218 167.3949 173.4832
2 C Isotropic = 147.6784 Anisotropy = 31.4153
XX= 160.0889 YX= -14.8127 ZX= 10.7714
XY= -7.7331 YY= 139.4946 ZY= -5.4684
XZ= 7.2659 YZ= -0.5427 ZZ= 143.4516
Eigenvalues: 134.3951 140.0181 168.6219
3 C Isotropic = 125.7364 Anisotropy = 54.1058
XX= 107.1220 YX= -26.8727 ZX= 35.7725
XY= -26.3876 YY= 132.7963 ZY= 11.4429
XZ= 30.3491 YZ= 3.7098 ZZ= 137.2908
Eigenvalues: 73.8088 141.5935 161.8069
4 C Isotropic = 123.4453 Anisotropy = 52.5703
XX= 121.9384 YX= -19.8881 ZX= 29.2194
XY= -22.9310 YY= 122.6094 ZY= -4.1456
XZ= 29.0508 YZ= 8.5196 ZZ= 125.7880

Eigenvalues: 86.0466 125.7970 158.4921
  5 C Isotropic = 38.8790 Anisotropy = 178.0772
XX= 25.3315 YX= -71.8430 ZX= -69.6212
XY= -76.4423 YY= 103.2085 ZY= -4.5610
XZ= -73.8204 YZ= 6.0166 ZZ= -11.9028
Eigenvalues: -79.8209 38.8609 157.5972
  6 C Isotropic = 56.7943 Anisotropy = 129.6888
XX= 53.7302 YX= -52.2418 ZX= -69.1568
XY= -35.9630 YY= 115.9988 ZY= -10.3812
XZ= -62.9684 YZ= -9.1532 ZZ= 0.6538
Eigenvalues: -50.7117 77.8410 143.2535
  7 C Isotropic = 104.9536 Anisotropy = 46.7526
XX= 122.8007 YX= -0.2579 ZX= -17.1653
XY= -3.7762 YY= 90.0185 ZY= 16.7616
XZ= -20.9655 YZ= 12.7442 ZZ= 102.0417
Eigenvalues: 77.8963 100.8425 136.1220
  8 C Isotropic = 136.1425 Anisotropy = 13.5434
XX= 140.6053 YX= -2.6793 ZX= -2.3790
XY= -7.9561 YY= 138.9143 ZY= -0.5598
XZ= 2.0740 YZ= 2.2442 ZZ= 128.9077
Eigenvalues: 128.8279 134.4281 145.1714
  9 C Isotropic = 152.3142 Anisotropy = 33.2281
XX= 165.8691 YX= -3.0789 ZX= 4.4584
XY= -6.4115 YY= 161.6091 ZY= -14.0805
XZ= 8.3295 YZ= -19.4592 ZZ= 129.4643
Eigenvalues: 121.9323 160.5440 174.4663
  10 C Isotropic = 142.7945 Anisotropy = 21.8110
XX= 151.1034 YX= 4.8908 ZX= 11.1865
XY= 2.8677 YY= 137.8138 ZY= 6.9334
XZ= 6.8365 YZ= 0.0411 ZZ= 139.4663
Eigenvalues: 134.0058 137.0426 157.3352
  11 O Isotropic = 95.5740 Anisotropy = 168.3771
XX= 67.2530 YX= 86.5157 ZX= 153.2502
XY= 71.1937 YY= 154.5333 ZY= -40.5531
XZ= 94.3761 YZ= -63.3391 ZZ= 64.9357
Eigenvalues: -92.4773 171.3739 207.8254
  12 C Isotropic = 13.4182 Anisotropy = 78.0728
XX= 31.9923 YX= -50.2534 ZX= -42.4003
XY= -45.3598 YY= -2.8906 ZY= -49.5268
XZ= -22.0421 YZ= -45.2761 ZZ= 11.1529
Eigenvalues: -74.6290 49.4168 65.4668
  13 C Isotropic = 32.7598 Anisotropy = 152.8175
XX= 2.9921 YX= 46.2756 ZX= 45.4381
XY= 47.8970 YY= 70.0207 ZY= -78.4506
XZ= 24.8802 YZ= -84.9278 ZZ= 25.2664
Eigenvalues: -77.4022 41.0433 134.6381
  14 O Isotropic = 260.5729 Anisotropy = 154.6673
XX= 332.9543 YX= -7.3104 ZX= 18.5032
XY= -1.7078 YY= 141.6480 ZY= -101.0290
XZ= 23.5692 YZ= -86.0320 ZZ= 307.1165
Eigenvalues: 99.4221 318.6122 363.6845
  15 O Isotropic = -66.4229 Anisotropy = 595.1235
XX= -303.4843 YX= -86.0864 ZX= 77.5138
XY= -113.6793 YY= 70.5085 ZY= -242.1240
XZ= 112.9036 YZ= -252.8711 ZZ= 33.7071

Eigenvalues: -333.5445 -196.0503 330.3261
16 C Isotropic = 61.8362 Anisotropy = 163.5389
XX= 8.3556 YX= 44.0904 ZX= 33.7099
XY= 50.1847 YY= 94.0757 ZY= -84.7482
XZ= 29.8121 YZ= -77.1852 ZZ= 83.0772
Eigenvalues: -47.8737 62.5201 170.8621
17 C Isotropic = 168.7233 Anisotropy = 33.1395
XX= 162.1984 YX= -2.7747 ZX= -0.0207
XY= -3.0704 YY= 159.6621 ZY= -13.4211
XZ= 4.3494 YZ= -14.1174 ZZ= 184.3093
Eigenvalues: 153.1444 162.2091 190.8163
18 C Isotropic = 168.3232 Anisotropy = 27.4819
XX= 158.2648 YX= -8.5993 ZX= 11.3867
XY= -5.8678 YY= 170.3439 ZY= -6.7671
XZ= 14.3593 YZ= -2.7020 ZZ= 176.3610
Eigenvalues: 150.5816 167.7436 186.6445
19 H Isotropic = 29.2221 Anisotropy = 9.2023
XX= 33.7899 YX= -2.9381 ZX= 1.9876
XY= -2.9296 YY= 28.4325 ZY= -0.9257
XZ= 0.4925 YZ= -1.5828 ZZ= 25.4440
Eigenvalues: 24.9831 27.3263 35.3570
20 H Isotropic = 29.8000 Anisotropy = 8.4926
XX= 30.6613 YX= 1.0303 ZX= -5.1563
XY= 0.4800 YY= 27.6256 ZY= -0.2769
XZ= -3.8230 YZ= -0.4608 ZZ= 31.1130
Eigenvalues: 26.3223 27.6159 35.4617
21 H Isotropic = 30.3735 Anisotropy = 6.2337
XX= 29.0546 YX= -1.4954 ZX= 2.4047
XY= -0.4228 YY= 29.4062 ZY= -0.6602
XZ= 2.9414 YZ= -1.7481 ZZ= 32.6596
Eigenvalues: 27.5794 29.0118 34.5293
22 H Isotropic = 29.9000 Anisotropy = 8.4677
XX= 32.1975 YX= 3.5040 ZX= 0.5946
XY= 3.3172 YY= 31.2815 ZY= 1.1840
XZ= 1.8606 YZ= 1.6069 ZZ= 26.2211
Eigenvalues: 25.8340 28.3209 35.5452
23 H Isotropic = 29.2245 Anisotropy = 7.9067
XX= 28.0446 YX= -1.9213 ZX= 4.1473
XY= 0.5408 YY= 32.4956 ZY= -2.5564
XZ= 1.0550 YZ= -3.8616 ZZ= 27.1333
Eigenvalues: 24.3677 28.8101 34.4956
24 H Isotropic = 25.8656 Anisotropy = 4.2116
XX= 25.9886 YX= 1.6372 ZX= -3.5232
XY= 1.4893 YY= 27.0313 ZY= 0.4724
XZ= -2.0617 YZ= 0.9119 ZZ= 24.5768
Eigenvalues: 21.9466 26.9768 28.6733
25 H Isotropic = 27.9593 Anisotropy = 5.3471
XX= 29.7636 YX= 0.8031 ZX= -1.0100
XY= 1.2680 YY= 26.7759 ZY= -2.8251
XZ= -1.3291 YZ= -3.3112 ZZ= 27.3385
Eigenvalues: 23.9760 28.3779 31.5241
26 H Isotropic = 29.0963 Anisotropy = 3.9383
XX= 28.7460 YX= -0.1908 ZX= 0.4060
XY= 0.8233 YY= 26.8793 ZY= -0.5149
XZ= 0.0494 YZ= 1.3513 ZZ= 31.6637

Eigenvalues: 26.7979 28.7692 31.7219
27 H Isotropic = 30.4037 Anisotropy = 8.5102
XX= 34.6323 YX= 2.6711 ZX= 0.3964
XY= 1.8376 YY= 32.4014 ZY= -1.1821
XZ= -0.0346 YZ= -2.1241 ZZ= 24.1774
Eigenvalues: 23.8218 31.3121 36.0772
28 H Isotropic = 29.5024 Anisotropy = 3.1592
XX= 29.0425 YX= -0.5569 ZX= -0.5866
XY= -1.6308 YY= 28.5666 ZY= -1.3181
XZ= 0.8893 YZ= -1.2413 ZZ= 30.8980
Eigenvalues: 27.4258 29.4729 31.6085
29 H Isotropic = 29.5814 Anisotropy = 6.3338
XX= 28.8317 YX= 0.0911 ZX= 0.2062
XY= 0.2564 YY= 29.2824 ZY= 4.7336
XZ= -0.1515 YZ= 2.8356 ZZ= 30.6301
Eigenvalues: 26.1072 28.8331 33.8040
30 H Isotropic = 29.5015 Anisotropy = 8.1151
XX= 28.2894 YX= -0.6550 ZX= 0.3976
XY= -0.2833 YY= 34.7141 ZY= -1.4564
XZ= 1.5282 YZ= -0.8745 ZZ= 25.5009
Eigenvalues: 25.1003 28.4925 34.9115
31 H Isotropic = 26.0907 Anisotropy = 7.3166
XX= 28.2056 YX= 2.8795 ZX= 4.1614
XY= 1.4788 YY= 24.3182 ZY= -0.2047
XZ= 2.2675 YZ= 0.5379 ZZ= 25.7484
Eigenvalues: 22.5886 24.7151 30.9685
32 H Isotropic = 25.2880 Anisotropy = 5.3749
XX= 26.3311 YX= 1.3778 ZX= 1.6533
XY= 2.8692 YY= 24.2747 ZY= 0.4297
XZ= 2.4887 YZ= 0.7685 ZZ= 25.2583
Eigenvalues: 22.7316 24.2612 28.8713
33 H Isotropic = 30.3559 Anisotropy = 6.7921
XX= 26.8446 YX= -0.5377 ZX= -0.1890
XY= -0.0462 YY= 29.8207 ZY= 0.6309
XZ= -1.4235 YZ= 2.1565 ZZ= 34.4024
Eigenvalues: 26.7521 29.4316 34.8840
34 H Isotropic = 30.4928 Anisotropy = 9.9981
XX= 30.4821 YX= 3.2987 ZX= -1.0559
XY= 4.2131 YY= 31.6427 ZY= -3.6856
XZ= -2.8659 YZ= -4.0268 ZZ= 29.3535
Eigenvalues: 26.2592 28.0609 37.1582
35 H Isotropic = 30.9068 Anisotropy = 9.1435
XX= 32.1509 YX= -2.5122 ZX= 1.8749
XY= -2.2523 YY= 29.9503 ZY= -4.4671
XZ= 1.9920 YZ= -5.1260 ZZ= 30.6193
Eigenvalues: 25.4454 30.2727 37.0025
36 H Isotropic = 29.6925 Anisotropy = 5.4265
XX= 31.3137 YX= 2.1516 ZX= 1.8561
XY= 1.8621 YY= 28.6210 ZY= -2.7053
XZ= 3.8057 YZ= -1.7060 ZZ= 29.1427
Eigenvalues: 24.8620 30.9052 33.3101
37 H Isotropic = 30.4282 Anisotropy = 10.9405
XX= 27.7340 YX= -2.5949 ZX= 2.5288
XY= -1.7433 YY= 35.1148 ZY= -3.8942
XZ= 1.5829 YZ= -3.9148 ZZ= 28.4356

Eigenvalues: 25.8460 27.7167 37.7218
38 H Isotropic = 30.1243 Anisotropy = 4.7350
XX= 29.9848 YX= -1.5442 ZX= -1.2803
XY= -2.1462 YY= 28.0739 ZY= 0.5874
XZ= -1.6506 YZ= 0.0662 ZZ= 32.3142
Eigenvalues: 26.9043 30.1877 33.2810

RRRSE

1 C Isotropic = 161.9618 Anisotropy = 19.1112
XX= 162.5944 YX= -6.1752 ZX= -8.3839
XY= -3.3248 YY= 166.4429 ZY= -12.0878
XZ= -6.5902 YZ= -12.1810 ZZ= 156.8481
Eigenvalues: 144.3028 166.8800 174.7026
2 C Isotropic = 145.6014 Anisotropy = 34.8108
XX= 166.1882 YX= 12.8777 ZX= 2.2822
XY= 6.3070 YY= 133.3180 ZY= 3.9591
XZ= -0.2146 YZ= -4.6871 ZZ= 137.2979
Eigenvalues: 130.6651 137.3305 168.8086
3 C Isotropic = 120.8974 Anisotropy = 54.3737
XX= 128.1835 YX= 32.1678 ZX= 29.6170
XY= 30.5074 YY= 119.1024 ZY= -23.2513
XZ= 24.7161 YZ= -19.1327 ZZ= 115.4064
Eigenvalues: 67.7458 137.7999 157.1466
4 C Isotropic = 120.9199 Anisotropy = 51.8869
XX= 140.3524 YX= 17.4784 ZX= 18.2699
XY= 28.2902 YY= 109.2931 ZY= -11.3701
XZ= 19.7957 YZ= -16.7066 ZZ= 113.1143
Eigenvalues: 81.8881 125.3605 155.5112
5 C Isotropic = 40.1886 Anisotropy = 176.9714
XX= -12.9005 YX= 55.5570 ZX= -72.9455
XY= 66.0835 YY= 95.3132 ZY= -19.1537
XZ= -88.0196 YZ= -40.0209 ZZ= 38.1531
Eigenvalues: -78.3249 40.7212 158.1695
6 C Isotropic = 54.5163 Anisotropy = 158.4904
XX= 8.8324 YX= 54.7076 ZX= -88.3241
XY= 45.9340 YY= 92.3882 ZY= -25.7553
XZ= -87.6412 YZ= -13.3978 ZZ= 62.3281
Eigenvalues: -62.1455 65.5177 160.1765
7 C Isotropic = 106.6122 Anisotropy = 46.6919
XX= 111.4214 YX= 11.4824 ZX= 20.1330
XY= 10.2345 YY= 111.2838 ZY= 19.2944
XZ= 17.3698 YZ= 14.1748 ZZ= 97.1314
Eigenvalues: 81.5468 100.5497 137.7401
8 C Isotropic = 134.4443 Anisotropy = 12.5895
XX= 138.9056 YX= 2.4033 ZX= 4.0536
XY= 9.5295 YY= 133.6231 ZY= -2.2862
XZ= -1.4278 YZ= -4.4250 ZZ= 130.8042
Eigenvalues: 126.6893 133.8063 142.8373
9 C Isotropic = 148.1269 Anisotropy = 38.0824
XX= 171.0435 YX= 7.2513 ZX= -0.2452
XY= 1.9566 YY= 137.4144 ZY= -12.3078
XZ= -11.5357 YZ= -16.6723 ZZ= 135.9228
Eigenvalues: 122.1336 148.7319 173.5151
10 C Isotropic = 149.4743 Anisotropy = 26.2832

XX= 166.8724 YX= -0.0151 ZX= -0.4388
XY= -2.0791 YY= 144.0245 ZY= 6.6899
XZ= 3.8588 YZ= 3.8878 ZZ= 137.5262
Eigenvalues: 134.4444 146.9821 166.9965
11 O Isotropic = 102.2473 Anisotropy = 170.5980
XX= 137.4115 YX= -131.6372 ZX= -89.3014
XY= -89.3046 YY= 59.4101 ZY= -93.2289
XZ= -51.8093 YZ= -119.7381 ZZ= 109.9202
Eigenvalues: -97.3934 188.1559 215.9793
12 C Isotropic = 13.8883 Anisotropy = 78.7546
XX= 18.9183 YX= 73.4056 ZX= 1.6886
XY= 58.7835 YY= -25.9725 ZY= 2.7821
XZ= -13.4306 YZ= 8.7426 ZZ= 48.7190
Eigenvalues: -73.8646 49.1381 66.3913
13 C Isotropic = 33.5244 Anisotropy = 150.5529
XX= 24.3883 YX= -40.3847 ZX= -36.2708
XY= -33.3080 YY= -27.4634 ZY= -63.9831
XZ= -16.2261 YZ= -73.1464 ZZ= 103.6483
Eigenvalues: -76.2630 42.9433 133.8930
14 O Isotropic = 261.4709 Anisotropy = 151.1280
XX= 346.3389 YX= 28.5167 ZX= 2.8271
XY= 15.3940 YY= 177.0432 ZY= 118.1797
XZ= 19.5208 YZ= 91.3533 ZZ= 261.0306
Eigenvalues: 105.5720 316.6178 362.2229
15 O Isotropic = -66.6075 Anisotropy = 590.8716
XX= -195.5116 YX= 56.0365 ZX= -234.4963
XY= 54.7068 YY= -158.3223 ZY= -119.1646
XZ= -274.9673 YZ= -134.0996 ZZ= 154.0114
Eigenvalues: -330.3771 -196.7523 327.3069
16 C Isotropic = 60.2644 Anisotropy = 166.1750
XX= 28.9418 YX= -41.6759 ZX= -40.7819
XY= -42.7527 YY= 3.2373 ZY= -59.2270
XZ= -35.6472 YZ= -50.3709 ZZ= 148.6141
Eigenvalues: -50.4450 60.1905 171.0477
17 C Isotropic = 168.1646 Anisotropy = 31.4947
XX= 167.1879 YX= 6.0409 ZX= 6.1045
XY= 6.4547 YY= 165.9305 ZY= 16.7197
XZ= 10.3302 YZ= 14.1402 ZZ= 171.3753
Eigenvalues: 152.9620 162.3707 189.1610
18 C Isotropic = 164.1793 Anisotropy = 29.5692
XX= 172.2716 YX= 7.3788 ZX= 11.9575
XY= 9.2405 YY= 155.2130 ZY= 3.0277
XZ= 13.9197 YZ= -1.4538 ZZ= 165.0533
Eigenvalues: 149.9694 158.6763 183.8920
19 H Isotropic = 29.2368 Anisotropy = 9.1502
XX= 34.3386 YX= 2.5009 ZX= -0.9895
XY= 2.1278 YY= 28.0073 ZY= -0.1626
XZ= -2.3860 YZ= 0.5078 ZZ= 25.3645
Eigenvalues: 24.9246 27.4488 35.3369
20 H Isotropic = 29.6337 Anisotropy = 8.4071
XX= 28.1473 YX= -1.5734 ZX= -3.7531
XY= -0.7845 YY= 28.0029 ZY= 1.8856
XZ= -2.6444 YZ= 2.4743 ZZ= 32.7508
Eigenvalues: 26.5040 27.1586 35.2384
21 H Isotropic = 30.4808 Anisotropy = 6.2152

XX= 31.2200 YX= 2.4057 ZX= 2.5821
XY= 1.3803 YY= 29.5356 ZY= 0.4207
XZ= 3.3989 YZ= 0.8531 ZZ= 30.6868
Eigenvalues: 27.5163 29.3018 34.6242
22 H Isotropic = 29.8967 Anisotropy = 8.0982
XX= 31.5533 YX= -3.8641 ZX= -0.4015
XY= -3.1550 YY= 31.6607 ZY= -1.1923
XZ= 0.8429 YZ= -1.8719 ZZ= 26.4761
Eigenvalues: 25.9201 28.4744 35.2955
23 H Isotropic = 29.4925 Anisotropy = 8.6512
XX= 30.5767 YX= 4.3716 ZX= 3.0296
XY= 1.4880 YY= 32.5974 ZY= 0.7403
XZ= 1.3969 YZ= 1.9286 ZZ= 25.3034
Eigenvalues: 24.4880 28.7295 35.2600
24 H Isotropic = 25.6780 Anisotropy = 5.8151
XX= 24.6735 YX= -2.8705 ZX= -3.7114
XY= -1.7691 YY= 27.8600 ZY= 1.0437
XZ= -1.9857 YZ= -0.9163 ZZ= 24.5005
Eigenvalues: 21.3300 26.1491 29.5547
25 H Isotropic = 27.0594 Anisotropy = 5.2652
XX= 26.2293 YX= -0.2666 ZX= -2.3704
XY= -0.0340 YY= 24.9089 ZY= -0.4940
XZ= -0.3566 YZ= -1.1143 ZZ= 30.0399
Eigenvalues: 24.6831 25.9255 30.5695
26 H Isotropic = 29.0014 Anisotropy = 6.1406
XX= 28.2585 YX= -0.6320 ZX= -2.1855
XY= -1.1441 YY= 28.5500 ZY= 1.9216
XZ= -1.2659 YZ= 3.7717 ZZ= 30.1957
Eigenvalues: 26.3286 27.5804 33.0951
27 H Isotropic = 30.3166 Anisotropy = 8.4439
XX= 33.8931 YX= -1.7358 ZX= 2.1311
XY= -1.2677 YY= 29.9687 ZY= -3.8346
XZ= 1.9515 YZ= -4.7216 ZZ= 27.0879
Eigenvalues: 23.9486 31.0553 35.9459
28 H Isotropic = 29.5488 Anisotropy = 3.0210
XX= 29.3895 YX= -0.0610 ZX= -0.1062
XY= -0.4397 YY= 28.4372 ZY= 0.6834
XZ= -2.0577 YZ= 0.6590 ZZ= 30.8196
Eigenvalues: 28.2596 28.8240 31.5627
29 H Isotropic = 30.0910 Anisotropy = 4.9849
XX= 30.8067 YX= -0.3190 ZX= 0.6152
XY= 0.1464 YY= 31.2277 ZY= 3.7786
XZ= 0.8487 YZ= 2.8588 ZZ= 28.2386
Eigenvalues: 26.0021 30.8566 33.4143
30 H Isotropic = 29.0339 Anisotropy = 9.0781
XX= 28.0015 YX= 1.3117 ZX= -0.6321
XY= 0.1941 YY= 32.1220 ZY= -4.7709
XZ= -0.2784 YZ= -4.7858 ZZ= 26.9782
Eigenvalues: 24.1236 27.8922 35.0859
31 H Isotropic = 26.0706 Anisotropy = 7.3621
XX= 29.4738 YX= -4.3506 ZX= -0.9781
XY= -2.0031 YY= 24.1548 ZY= -0.3516
XZ= -0.1041 YZ= -0.2296 ZZ= 24.5832
Eigenvalues: 22.5510 24.6822 30.9787
32 H Isotropic = 25.2301 Anisotropy = 5.6106

XX= 27.0294 YX= -2.1922 ZX= -0.1584
XY= -3.6787 YY= 24.5311 ZY= -0.5451
XZ= -0.0803 YZ= 0.2233 ZZ= 24.1296
Eigenvalues: 22.5646 24.1552 28.9705
33 H Isotropic = 30.2978 Anisotropy = 5.7861
XX= 27.6590 YX= 0.1871 ZX= 2.0484
XY= 0.0549 YY= 29.3601 ZY= 0.4239
XZ= 0.5705 YZ= -1.0452 ZZ= 33.8741
Eigenvalues: 27.3779 29.3602 34.1552
34 H Isotropic = 30.5948 Anisotropy = 9.7833
XX= 29.4916 YX= -1.9220 ZX= -0.2299
XY= -3.1166 YY= 33.9338 ZY= 4.1264
XZ= -1.6548 YZ= 4.2653 ZZ= 28.3589
Eigenvalues: 26.0615 28.6059 37.1169
35 H Isotropic = 29.8224 Anisotropy = 9.1874
XX= 34.3808 YX= 2.8624 ZX= 0.0450
XY= 2.8206 YY= 29.2474 ZY= 3.2125
XZ= 0.3591 YZ= 3.9500 ZZ= 25.8390
Eigenvalues: 23.3995 30.1204 35.9473
36 H Isotropic = 29.6409 Anisotropy = 6.1871
XX= 33.2006 YX= -1.7428 ZX= 1.1371
XY= -0.1115 YY= 29.0859 ZY= 2.8046
XZ= 2.8102 YZ= 1.9500 ZZ= 26.6361
Eigenvalues: 24.6373 30.5197 33.7656
37 H Isotropic = 30.1589 Anisotropy = 10.1021
XX= 29.3391 YX= 4.1840 ZX= 1.9577
XY= 2.9763 YY= 34.8218 ZY= 1.4962
XZ= 0.9105 YZ= 1.0774 ZZ= 26.3159
Eigenvalues: 25.7408 27.8424 36.8937
38 H Isotropic = 30.4075 Anisotropy = 4.9023
XX= 28.8743 YX= 1.4918 ZX= -0.4390
XY= 1.2916 YY= 28.7975 ZY= 0.2264
XZ= -0.9001 YZ= 0.9148 ZZ= 33.5507
Eigenvalues: 27.3205 30.2263 33.6757

RSRRE

1 C Isotropic = 161.4270 Anisotropy = 17.1519
XX= 165.1970 YX= 0.0583 ZX= 1.2250
XY= 1.0119 YY= 167.8503 ZY= 9.1064
XZ= 0.3745 YZ= 11.4856 ZZ= 151.2337
Eigenvalues: 146.2991 165.1203 172.8616
2 C Isotropic = 150.4786 Anisotropy = 22.5142
XX= 148.2421 YX= -14.9387 ZX= 6.1842
XY= -6.6574 YY= 155.1196 ZY= -5.0157
XZ= 4.8125 YZ= -3.1322 ZZ= 148.0742
Eigenvalues: 139.7144 146.2335 165.4881
3 C Isotropic = 124.5601 Anisotropy = 55.5576
XX= 79.3811 YX= -12.9382 ZX= -4.4112
XY= -16.6184 YY= 148.4452 ZY= -14.9193
XZ= -3.8564 YZ= -12.1080 ZZ= 145.8540
Eigenvalues: 75.6805 136.4013 161.5985
4 C Isotropic = 120.8255 Anisotropy = 53.3682
XX= 86.3001 YX= -1.8969 ZX= -5.2742
XY= 4.2123 YY= 138.9861 ZY= -13.5098

XZ= -6.5916 YZ= -22.3813 ZZ= 137.1904
Eigenvalues: 85.6004 120.4719 156.4044
  5 C Isotropic = 40.2831 Anisotropy = 176.3665
XX= 53.7686 YX= -65.4848 ZX= -69.6123
XY= -69.9611 YY= 95.2972 ZY= -2.1471
XZ= -73.8430 YZ= 9.3806 ZZ= -28.2165
Eigenvalues: -76.1795 39.1681 157.8608
  6 C Isotropic = 55.2101 Anisotropy = 131.9147
XX= 72.8458 YX= -43.1469 ZX= -67.7796
XY= -31.2952 YY= 110.2944 ZY= 2.1975
XZ= -59.1760 YZ= 4.3334 ZZ= -17.5099
Eigenvalues: -51.5449 74.0220 143.1532
  7 C Isotropic = 102.9860 Anisotropy = 43.1125
XX= 115.0847 YX= -9.2137 ZX= -14.4028
XY= -7.7825 YY= 102.6358 ZY= 13.6120
XZ= -22.0043 YZ= 12.9381 ZZ= 91.2374
Eigenvalues: 78.4902 98.7401 131.7277
  8 C Isotropic = 138.4146 Anisotropy = 11.5010
XX= 145.6231 YX= 3.1821 ZX= 0.9558
XY= -4.7058 YY= 139.0015 ZY= 1.9905
XZ= 4.3553 YZ= 5.3664 ZZ= 130.6192
Eigenvalues: 128.7835 140.3784 146.0819
  9 C Isotropic = 146.9168 Anisotropy = 35.7064
XX= 151.1461 YX= -3.0693 ZX= 7.1467
XY= -4.4384 YY= 168.9356 ZY= -2.8696
XZ= 15.6147 YZ= -6.3719 ZZ= 120.6686
Eigenvalues: 116.6892 153.3401 170.7210
  10 C Isotropic = 143.0497 Anisotropy = 23.6559
XX= 147.8828 YX= 5.1023 ZX= 13.7605
XY= 3.7142 YY= 139.7652 ZY= 10.2373
XZ= 8.5969 YZ= 0.9350 ZZ= 141.5010
Eigenvalues: 132.4553 137.8734 158.8203
  11 O Isotropic = 90.6938 Anisotropy = 165.0082
XX= 55.3889 YX= 105.3988 ZX= 137.6723
XY= 81.5300 YY= 123.9871 ZY= -66.4043
XZ= 98.1017 YZ= -56.6089 ZZ= 92.7052
Eigenvalues: -100.3956 171.7776 200.6992
  12 C Isotropic = 13.4640 Anisotropy = 76.7643
XX= 24.9289 YX= -35.3655 ZX= -58.1302
XY= -31.9619 YY= 34.4314 ZY= -35.1132
XZ= -41.5025 YZ= -37.4637 ZZ= -18.9683
Eigenvalues: -73.5975 49.3492 64.6402
  13 C Isotropic = 36.9798 Anisotropy = 148.0781
XX= 22.7224 YX= 59.5003 ZX= 33.3510
XY= 62.4120 YY= 73.0640 ZY= -68.9751
XZ= 18.5302 YZ= -75.7827 ZZ= 15.1530
Eigenvalues: -69.9044 45.1453 135.6985
  14 O Isotropic = 252.9739 Anisotropy = 156.4693
XX= 307.2279 YX= 21.0812 ZX= 0.6367
XY= 22.6573 YY= 198.4701 ZY= -134.9810
XZ= 0.1422 YZ= -114.6164 ZZ= 253.2237
Eigenvalues: 96.6572 304.9777 357.2868
  15 O Isotropic = -60.5673 Anisotropy = 584.8584
XX= -305.4626 YX= 77.8220 ZX= -48.3042
XY= 63.6845 YY= 162.2963 ZY= -235.8465

XZ= -32.5491 YZ= -237.3850 ZZ= -38.5356
Eigenvalues: -316.1104 -194.9298 329.3383
 16 C Isotropic = 58.8429 Anisotropy = 170.1113
XX= 23.1181 YX= 64.8683 ZX= 21.0908
XY= 71.5469 YY= 95.7369 ZY= -81.5444
XZ= 21.1813 YZ= -80.0091 ZZ= 57.6739
Eigenvalues: -55.2834 59.5617 172.2505
 17 C Isotropic = 164.6069 Anisotropy = 39.6888
XX= 163.7483 YX= 5.1531 ZX= -10.5207
XY= 9.1132 YY= 160.8160 ZY= -21.6742
XZ= -6.5105 YZ= -20.5163 ZZ= 169.2565
Eigenvalues: 143.5222 159.2324 191.0661
 18 C Isotropic = 170.2300 Anisotropy = 26.4314
XX= 158.9334 YX= -10.7819 ZX= 6.8799
XY= -8.0673 YY= 171.6469 ZY= -7.6809
XZ= 11.4046 YZ= -2.3231 ZZ= 180.1097
Eigenvalues: 152.5785 170.2606 187.8510
 19 H Isotropic = 29.3443 Anisotropy = 8.5855
XX= 32.7231 YX= -2.4686 ZX= 3.4216
XY= -2.4139 YY= 29.4581 ZY= -1.5315
XZ= 1.5580 YZ= -2.2654 ZZ= 25.8518
Eigenvalues: 24.7486 28.2164 35.0680
 20 H Isotropic = 29.8004 Anisotropy = 7.7336
XX= 31.8898 YX= 1.0897 ZX= -4.6225
XY= 0.2821 YY= 28.2637 ZY= -0.4416
XZ= -3.4818 YZ= -0.7862 ZZ= 29.2478
Eigenvalues: 26.3020 28.1431 34.9561
 21 H Isotropic = 29.9115 Anisotropy = 8.4524
XX= 30.6865 YX= 2.0614 ZX= 3.1038
XY= 2.1057 YY= 30.6361 ZY= 2.3068
XZ= 4.5049 YZ= 2.6036 ZZ= 28.4120
Eigenvalues: 25.4464 28.7418 35.5465
 22 H Isotropic = 30.3090 Anisotropy = 4.8513
XX= 28.6905 YX= -0.5471 ZX= -0.2022
XY= -0.3298 YY= 30.5048 ZY= -1.9339
XZ= 0.0879 YZ= -2.7370 ZZ= 31.7318
Eigenvalues: 28.3101 29.0738 33.5432
 23 H Isotropic = 29.4809 Anisotropy = 6.7740
XX= 28.7085 YX= 3.2406 ZX= 2.1838
XY= 1.4374 YY= 29.4696 ZY= -4.5989
XZ= 4.9718 YZ= -2.8469 ZZ= 30.2647
Eigenvalues: 23.0467 31.3992 33.9969
 24 H Isotropic = 25.8732 Anisotropy = 4.6349
XX= 26.7906 YX= 2.1744 ZX= -3.1361
XY= 1.6713 YY= 26.9251 ZY= 1.1321
XZ= -1.7563 YZ= 1.4375 ZZ= 23.9040
Eigenvalues: 21.6667 26.9899 28.9632
 25 H Isotropic = 28.1152 Anisotropy = 6.5347
XX= 30.7191 YX= -2.1596 ZX= 0.3655
XY= -2.6450 YY= 29.1236 ZY= -0.6158
XZ= -0.4118 YZ= -0.7723 ZZ= 24.5028
Eigenvalues: 24.3741 27.4998 32.4717
 26 H Isotropic = 29.2061 Anisotropy = 2.0203
XX= 29.7319 YX= -0.2649 ZX= -0.3443
XY= 1.6635 YY= 27.8748 ZY= -1.1124

XZ= -0.4324 YZ=   0.0478 ZZ= 30.0115
Eigenvalues: 27.5780 29.4873 30.5529
 27 H Isotropic = 30.3136 Anisotropy =   8.5484
XX= 33.5567 YX=   2.4907 ZX=   2.8143
XY=   2.0693 YY= 31.8684 ZY=   2.0096
XZ=   2.4549 YZ=   0.9851 ZZ= 25.5158
Eigenvalues: 24.6356 30.2927 36.0126
 28 H Isotropic = 29.6472 Anisotropy =   4.5186
XX= 29.1622 YX=   0.6352 ZX= -1.9421
XY= -0.9705 YY= 29.6932 ZY= -2.3850
XZ= -0.7078 YZ= -2.6931 ZZ= 30.0861
Eigenvalues: 26.8606 29.4213 32.6596
 29 H Isotropic = 29.4522 Anisotropy =   8.3125
XX= 27.5129 YX= -0.8380 ZX=   0.4663
XY= -0.6094 YY= 34.9205 ZY= -0.0207
XZ=   1.4911 YZ=   0.5579 ZZ= 25.9233
Eigenvalues: 25.4246 27.9381 34.9938
 30 H Isotropic = 29.5653 Anisotropy =   6.7825
XX= 28.5961 YX=   0.1497 ZX=   0.0345
XY=   0.2432 YY= 28.1543 ZY=   4.5708
XZ= -0.6853 YZ=   2.5449 ZZ= 31.9454
Eigenvalues: 25.9754 28.6335 34.0869
 31 H Isotropic = 26.0360 Anisotropy =   7.5823
XX= 28.3832 YX=   1.4397 ZX=   4.7502
XY=   0.3228 YY= 23.9040 ZY= -1.3088
XZ=   2.7853 YZ= -0.2772 ZZ= 25.8209
Eigenvalues: 22.2887 24.7284 31.0909
 32 H Isotropic = 25.1171 Anisotropy =   5.5376
XX= 26.3530 YX=   0.6781 ZX=   1.9830
XY=   2.1408 YY= 23.4972 ZY=   0.0955
XZ=   3.2699 YZ= -0.1133 ZZ= 25.5011
Eigenvalues: 22.3696 24.1729 28.8088
 33 H Isotropic = 30.1093 Anisotropy =   8.0016
XX= 27.9863 YX= -1.2966 ZX= -3.5140
XY=   0.1089 YY= 28.8983 ZY= -0.6949
XZ= -4.1790 YZ=   0.7353 ZZ= 33.4433
Eigenvalues: 25.9087 28.9755 35.4437
 34 H Isotropic = 30.4428 Anisotropy = 10.1291
XX= 32.0965 YX=   4.4662 ZX=   0.5116
XY=   5.7112 YY= 31.8339 ZY= -1.0660
XZ= -1.1662 YZ= -1.6088 ZZ= 27.3980
Eigenvalues: 26.3171 27.8157 37.1955
 35 H Isotropic = 31.0957 Anisotropy = 10.2063
XX= 29.7217 YX= -1.3258 ZX=   0.9772
XY= -0.9103 YY= 32.2989 ZY= -5.7891
XZ=   1.3002 YZ= -5.7784 ZZ= 31.2663
Eigenvalues: 25.9738 29.4133 37.8999
 36 H Isotropic = 29.6739 Anisotropy =   5.4788
XX= 30.1764 YX=   2.5390 ZX=   2.2816
XY=   2.1390 YY= 29.2043 ZY= -2.3495
XZ=   4.3225 YZ= -1.0923 ZZ= 29.6411
Eigenvalues: 24.7546 30.9408 33.3265
 37 H Isotropic = 30.3951 Anisotropy = 11.0270
XX= 27.4244 YX= -2.9659 ZX=   2.3437
XY= -1.9049 YY= 35.7828 ZY= -3.1096

XZ= 1.4908 YZ= -3.2171 ZZ= 27.9781
Eigenvalues: 25.7552 27.6837 37.7464
38 H Isotropic = 30.0594 Anisotropy = 4.8488
XX= 30.7510 YX= -1.2164 ZX= -1.6192
XY= -1.8978 YY= 27.5556 ZY= -0.1158
XZ= -2.0475 YZ= -0.7654 ZZ= 31.8717
Eigenvalues: 26.6659 30.2205 33.2920

RRSSZ

1 C Isotropic = 159.4348 Anisotropy = 17.5105
XX= 161.5524 YX= -3.0698 ZX= -9.9422
XY= -0.8155 YY= 170.5535 ZY= -3.9240
XZ= -8.3837 YZ= -3.0142 ZZ= 146.1985
Eigenvalues: 141.3825 165.8134 171.1085
2 C Isotropic = 147.2307 Anisotropy = 28.9560
XX= 154.2428 YX= -12.4220 ZX= 13.9205
XY= -5.9018 YY= 138.1215 ZY= -2.5000
XZ= 10.0783 YZ= -1.3896 ZZ= 149.3279
Eigenvalues: 133.0513 142.1062 166.5347
3 C Isotropic = 125.4537 Anisotropy = 55.2107
XX= 102.9287 YX= -21.7952 ZX= 36.1184
XY= -18.7594 YY= 130.8792 ZY= 12.4756
XZ= 31.6587 YZ= 4.8232 ZZ= 142.5531
Eigenvalues: 74.9107 139.1896 162.2608
4 C Isotropic = 120.4019 Anisotropy = 54.0280
XX= 112.5709 YX= -7.5767 ZX= 33.5766
XY= -12.0535 YY= 120.0185 ZY= -7.5384
XZ= 34.5542 YZ= 9.2480 ZZ= 128.6162
Eigenvalues: 83.7115 121.0736 156.4205
5 C Isotropic = 40.7915 Anisotropy = 170.0476
XX= 89.7867 YX= -54.9311 ZX= -21.8118
XY= -47.6734 YY= 40.8590 ZY= 88.5877
XZ= -25.2185 YZ= 85.0161 ZZ= -8.2713
Eigenvalues: -74.9213 43.1392 154.1566
6 C Isotropic = 53.0005 Anisotropy = 122.3284
XX= 95.2913 YX= -19.7597 ZX= -18.5499
XY= -27.7587 YY= 69.7637 ZY= 70.9001
XZ= -17.2286 YZ= 70.8770 ZZ= -6.0534
Eigenvalues: -48.6038 73.0526 134.5528
7 C Isotropic = 103.6950 Anisotropy = 48.0948
XX= 117.5976 YX= -9.5181 ZX= -14.2340
XY= -15.5172 YY= 106.4015 ZY= 18.9910
XZ= -16.4210 YZ= 14.3132 ZZ= 87.0859
Eigenvalues: 75.9967 99.3301 135.7582
8 C Isotropic = 140.9799 Anisotropy = 21.6139
XX= 148.6922 YX= 6.0235 ZX= -7.4876
XY= 6.0047 YY= 145.3844 ZY= -1.5360
XZ= -7.3346 YZ= -3.5234 ZZ= 128.8630
Eigenvalues: 126.3846 141.1658 155.3891

9 C Isotropic = 158.0021 Anisotropy = 18.0347
XX= 164.1579 YX= -7.6771 ZX= -1.8045
XY= -7.7315 YY= 150.2393 ZY= 7.1113
XZ= 0.1163 YZ= 10.6263 ZZ= 159.6090
Eigenvalues: 143.0085 160.9725 170.0252
10 C Isotropic = 156.4061 Anisotropy = 13.4439
XX= 156.2161 YX= -12.3078 ZX= 1.9838
XY= -7.5110 YY= 149.2951 ZY= 1.7234
XZ= 1.1367 YZ= -3.8073 ZZ= 163.7069
Eigenvalues: 142.2592 161.5903 165.3687
11 O Isotropic = 91.6597 Anisotropy = 162.4363
XX= 32.2426 YX= 142.3351 ZX= 92.9308
XY= 107.8084 YY= 106.6739 ZY= -43.5780
XZ= 51.4372 YZ= -63.5867 ZZ= 136.0628
Eigenvalues: -95.8764 170.9050 199.9506
12 C Isotropic = 13.4713 Anisotropy = 77.4362
XX= 39.2777 YX= -59.9714 ZX= -12.2707
XY= -47.1287 YY= -46.4283 ZY= -18.8422
XZ= -0.8052 YZ= -13.6406 ZZ= 47.5645
Eigenvalues: -74.6583 49.9768 65.0955
13 C Isotropic = 37.5902 Anisotropy = 142.6175
XX= -2.1301 YX= 55.2121 ZX= 15.9674
XY= 54.0976 YY= 1.4926 ZY= -51.1301
XZ= 9.2673 YZ= -47.8917 ZZ= 113.4083
Eigenvalues: -65.9161 46.0182 132.6686
14 O Isotropic = 260.7248 Anisotropy = 158.1959
XX= 333.3671 YX= 11.4070 ZX= 25.2820
XY= 19.9244 YY= 113.9316 ZY= -51.1194
XZ= 32.5143 YZ= -52.2747 ZZ= 334.8757
Eigenvalues: 100.4156 315.5701 366.1888
15 O Isotropic = -65.2575 Anisotropy = 583.5333
XX= -292.6107 YX= -42.0995 ZX= 109.7656
XY= -48.0611 YY= -159.4125 ZY= -130.3987
XZ= 142.7425 YZ= -133.8946 ZZ= 256.2506
Eigenvalues: -322.1578 -197.3794 323.7646
16 C Isotropic = 62.8095 Anisotropy = 171.7065
XX= 2.4492 YX= 53.6501 ZX= 15.8007
XY= 54.8640 YY= 29.9206 ZY= -56.3186
XZ= 5.4673 YZ= -53.9250 ZZ= 156.0587
Eigenvalues: -48.9956 60.1437 177.2805
17 C Isotropic = 169.0436 Anisotropy = 28.8678
XX= 163.2553 YX= 0.2136 ZX= -3.7620
XY= 1.2024 YY= 157.9444 ZY= -8.9031
XZ= 0.5344 YZ= -7.5397 ZZ= 185.9310
Eigenvalues: 155.6990 163.1430 188.2887
18 C Isotropic = 163.2225 Anisotropy = 35.9515
XX= 151.0069 YX= 9.2470 ZX= -3.9165
XY= 8.8006 YY= 176.2866 ZY= -13.5506

XZ= -3.9944 YZ= -13.5279 ZZ= 162.3740
Eigenvalues: 148.0995 154.3778 187.1902
 19 H Isotropic = 29.7025 Anisotropy = 10.9948
XX= 36.3667 YX= -1.5058 ZX= 2.4107
XY= -1.8811 YY= 28.3284 ZY= -1.1095
XZ= 1.1956 YZ= -1.3800 ZZ= 24.4124
Eigenvalues: 23.9127 28.1625 37.0324
 20 H Isotropic = 29.4496 Anisotropy = 4.4244
XX= 29.4996 YX= 0.2134 ZX= -3.2509
XY= -1.0966 YY= 28.5434 ZY= 0.9312
XZ= -1.1866 YZ= 0.8419 ZZ= 30.3059
Eigenvalues: 27.5788 28.3708 32.3993
 21 H Isotropic = 30.7307 Anisotropy = 8.2588
XX= 29.2684 YX= -0.6610 ZX= 2.9262
XY= -0.3880 YY= 28.4551 ZY= 1.5981
XZ= 3.6940 YZ= 1.3608 ZZ= 34.4687
Eigenvalues: 26.8248 29.1307 36.2366
 22 H Isotropic = 29.8131 Anisotropy = 8.6042
XX= 32.6718 YX= 3.5482 ZX= 0.7226
XY= 3.3309 YY= 31.1948 ZY= -0.4514
XZ= 2.1289 YZ= 0.0440 ZZ= 25.5726
Eigenvalues: 25.1398 28.7502 35.5492
 23 H Isotropic = 29.0745 Anisotropy = 5.4828
XX= 27.3350 YX= -0.1354 ZX= 4.0115
XY= 1.5978 YY= 30.0063 ZY= -2.2267
XZ= -0.0489 YZ= -3.0277 ZZ= 29.8821
Eigenvalues: 25.3455 29.1482 32.7297
 24 H Isotropic = 26.0770 Anisotropy = 4.6843
XX= 27.5514 YX= 1.3670 ZX= 2.0714
XY= 2.2785 YY= 27.1198 ZY= -0.8130
XZ= 1.1797 YZ= -1.7606 ZZ= 23.5598
Eigenvalues: 22.2561 26.7751 29.1999
 25 H Isotropic = 28.1293 Anisotropy = 4.1461
XX= 30.0233 YX= -0.0314 ZX= -1.1005
XY= 0.0870 YY= 26.1828 ZY= -0.8563
XZ= -1.7653 YZ= -1.6264 ZZ= 28.1818
Eigenvalues: 25.5005 27.9940 30.8934
 26 H Isotropic = 29.0567 Anisotropy = 3.4901
XX= 29.5554 YX= -0.4589 ZX= -0.1626
XY= -1.8843 YY= 28.6407 ZY= -1.6839
XZ= 1.6433 YZ= -1.4669 ZZ= 28.9741
Eigenvalues: 27.1473 28.6394 31.3835
 27 H Isotropic = 30.3441 Anisotropy = 7.4245
XX= 30.1370 YX= -0.3803 ZX= 2.9706
XY= 0.4418 YY= 26.8041 ZY= 0.2560
XZ= 1.9600 YZ= 0.6161 ZZ= 34.0912
Eigenvalues: 26.7728 28.9658 35.2938
 28 H Isotropic = 29.4263 Anisotropy = 7.4706

XX= 30.6733 YX= 2.2867 ZX= 0.4259
XY= 1.9557 YY= 32.9424 ZY= 0.9450
XZ= 1.1661 YZ= 1.2997 ZZ= 24.6631
Eigenvalues: 24.4677 29.4045 34.4066
29 H Isotropic = 29.1207 Anisotropy = 7.8623
XX= 29.4583 YX= 3.3404 ZX= 0.4729
XY= 3.5629 YY= 31.8134 ZY= -0.0069
XZ= -1.5134 YZ= -1.2413 ZZ= 26.0903
Eigenvalues: 26.0073 26.9925 34.3622
30 H Isotropic = 29.7483 Anisotropy = 9.7677
XX= 29.1137 YX= -2.6950 ZX= -2.8857
XY= -1.8486 YY= 29.3888 ZY= 4.8333
XZ= -1.6153 YZ= 4.6118 ZZ= 30.7425
Eigenvalues: 25.2737 27.7111 36.2602
31 H Isotropic = 26.2294 Anisotropy = 7.9876
XX= 29.3756 YX= 4.8442 ZX= 1.4023
XY= 2.4639 YY= 24.8745 ZY= -0.0514
XZ= 0.6219 YZ= 0.4869 ZZ= 24.4381
Eigenvalues: 22.7742 24.3596 31.5544
32 H Isotropic = 25.2204 Anisotropy = 5.1814
XX= 26.1234 YX= 1.9856 ZX= 0.3678
XY= 3.6219 YY= 25.3221 ZY= 0.5661
XZ= 0.4414 YZ= 0.7283 ZZ= 24.2155
Eigenvalues: 22.8511 24.1353 28.6746
33 H Isotropic = 30.8641 Anisotropy = 8.0966
XX= 32.2846 YX= -0.0591 ZX= 2.8358
XY= -0.0009 YY= 27.4983 ZY= -3.4079
XZ= 2.8069 YZ= -3.6815 ZZ= 32.8093
Eigenvalues: 25.4746 30.8558 36.2618
34 H Isotropic = 30.0457 Anisotropy = 6.7961
XX= 27.5941 YX= -1.6181 ZX= -2.0837
XY= -1.5603 YY= 30.1042 ZY= 0.9050
XZ= -3.5072 YZ= 1.9145 ZZ= 32.4389
Eigenvalues: 26.1063 29.4544 34.5765
35 H Isotropic = 30.3105 Anisotropy = 10.6793
XX= 28.7489 YX= 3.8338 ZX= -1.1337
XY= 4.2939 YY= 32.7751 ZY= -3.3175
XZ= -2.8457 YZ= -3.9468 ZZ= 29.4075
Eigenvalues: 26.1892 27.3123 37.4300
36 H Isotropic = 30.0044 Anisotropy = 7.7784
XX= 28.2485 YX= 0.3483 ZX= 1.7575
XY= -0.6145 YY= 30.0127 ZY= -4.3194
XZ= 3.3619 YZ= -2.7675 ZZ= 31.7521
Eigenvalues: 25.9880 28.8352 35.1900
37 H Isotropic = 30.1703 Anisotropy = 9.4063
XX= 26.6711 YX= -0.8889 ZX= 0.6282
XY= 0.1895 YY= 36.1972 ZY= 1.9307
XZ= 0.3231 YZ= 0.9539 ZZ= 27.6427

Eigenvalues: 26.3912 27.6785 36.4412
38 H Isotropic = 29.9099 Anisotropy = 4.9539
XX= 32.7051 YX= -0.1188 ZX= -1.0136
XY= -0.0899 YY= 29.0661 ZY= -3.0066
XZ= -1.4816 YZ= -3.5127 ZZ= 27.9585
Eigenvalues: 25.0681 31.4491 33.2125

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1 C Isotropic = 158.7445 Anisotropy = 18.9806
XX= 155.9705 YX= -10.4140 ZX= -10.1887
XY= -12.2936 YY= 161.9162 ZY= -4.0223
XZ= -9.6520 YZ= -5.0959 ZZ= 158.3468
Eigenvalues: 140.7140 164.1213 171.3983
2 C Isotropic = 147.3016 Anisotropy = 30.9282
XX= 167.7782 YX= -2.8359 ZX= 4.4421
XY= 2.4121 YY= 132.5786 ZY= 2.1808
XZ= -0.5697 YZ= 3.4888 ZZ= 141.5479
Eigenvalues: 131.7424 142.2420 167.9204
3 C Isotropic = 126.8037 Anisotropy = 59.3185
XX= 158.1925 YX= -13.4247 ZX= 22.4069
XY= -7.7895 YY= 112.3407 ZY= 33.5499
XZ= 20.3899 YZ= 29.4517 ZZ= 109.8779
Eigenvalues: 73.4114 140.6503 166.3493
4 C Isotropic = 126.2652 Anisotropy = 52.9285
XX= 158.8527 YX= 0.5643 ZX= 11.3117
XY= -13.3937 YY= 113.0901 ZY= 21.9294
XZ= 12.9113 YZ= 29.0128 ZZ= 106.8529
Eigenvalues: 81.9955 135.2492 161.5509
5 C Isotropic = 42.9267 Anisotropy = 167.8310
XX= 76.0601 YX= -28.2906 ZX= -82.4065
XY= -20.7428 YY= 61.5317 ZY= 58.1750
XZ= -82.1572 YZ= 53.7077 ZZ= -8.8115
Eigenvalues: -69.3385 43.3046 154.8141
6 C Isotropic = 51.1019 Anisotropy = 124.3204
XX= 58.1810 YX= -11.5643 ZX= -73.4614
XY= -15.8660 YY= 87.0376 ZY= 34.5528
XZ= -72.4228 YZ= 38.5860 ZZ= 8.0872
Eigenvalues: -47.6967 67.0203 133.9822
7 C Isotropic = 104.3561 Anisotropy = 48.4432
XX= 117.8000 YX= -22.4908 ZX= 0.2705
XY= -21.4457 YY= 110.6980 ZY= 3.9037
XZ= 4.4226 YZ= 10.1218 ZZ= 84.5702
Eigenvalues: 80.3816 96.0351 136.6516
8 C Isotropic = 135.0713 Anisotropy = 8.8444
XX= 139.2679 YX= -3.8017 ZX= 3.2639
XY= -3.3946 YY= 129.3626 ZY= -2.4127

XZ= -6.3407 YZ=   2.8071 ZZ= 136.5835
Eigenvalues: 128.1834 136.0630 140.9676
  9 C Isotropic = 160.1548 Anisotropy = 16.7351
XX= 166.0048 YX= -6.5137 ZX= -3.5306
XY= -5.3539 YY= 163.6463 ZY= -0.9397
XZ= -6.0684 YZ= -1.6329 ZZ= 150.8133
Eigenvalues: 148.7987 160.3541 171.3116
  10 C Isotropic = 151.6268 Anisotropy = 20.8742
XX= 161.6402 YX= -11.1789 ZX=   2.3598
XY= -8.3875 YY= 140.6663 ZY=   5.1650
XZ= -0.7575 YZ=   3.1006 ZZ= 152.5738
Eigenvalues: 135.7897 153.5477 165.5429
  11 O Isotropic = 94.8077 Anisotropy = 167.8031
XX= -2.8141 YX= 170.6175 ZX= 29.1849
XY= 111.8738 YY= 96.1563 ZY= -20.3927
XZ= 33.7638 YZ=   3.7285 ZZ= 191.0808
Eigenvalues: -106.1253 183.8719 206.6764
  12 C Isotropic = 13.4424 Anisotropy = 78.2187
XX= 49.7208 YX= -40.9165 ZX= -29.7910
XY= -22.5250 YY= -19.7888 ZY= -50.0437
XZ= -28.8712 YZ= -57.9767 ZZ= 10.3952
Eigenvalues: -75.5518 50.2908 65.5882
  13 C Isotropic = 37.9201 Anisotropy = 141.0432
XX= -15.5386 YX= 51.1212 ZX= 27.3087
XY= 45.4681 YY= 22.1725 ZY= -51.5618
XZ= 34.1356 YZ= -51.7701 ZZ= 107.1266
Eigenvalues: -66.2100 48.0214 131.9490
  14 O Isotropic = 260.1385 Anisotropy = 164.6114
XX= 350.8414 YX= 37.8842 ZX= 34.4261
XY= 60.7436 YY= 139.2961 ZY= -85.0984
XZ= 40.7117 YZ= -62.1174 ZZ= 290.2780
Eigenvalues: 95.2760 315.2600 369.8794
  15 O Isotropic = -68.5971 Anisotropy = 586.1453
XX= -289.8167 YX= 42.9162 ZX= -114.4294
XY= 66.0784 YY= -66.3336 ZY= -222.6637
XZ= -145.8826 YZ= -224.4470 ZZ= 150.3588
Eigenvalues: -325.6870 -202.2708 322.1664
  16 C Isotropic = 62.8023 Anisotropy = 172.7912
XX= -10.7455 YX= 46.4481 ZX= 27.0526
XY= 38.3092 YY= 52.3005 ZY= -59.7020
XZ= 37.5060 YZ= -63.9177 ZZ= 146.8517
Eigenvalues: -49.5491 59.9595 177.9964
  17 C Isotropic = 167.9925 Anisotropy = 24.1746
XX= 172.8328 YX= -0.6302 ZX= 7.7800
XY= -1.5817 YY= 158.7346 ZY= -12.3811
XZ= 11.1929 YZ= -5.1423 ZZ= 172.4102
Eigenvalues: 153.8101 166.0586 184.1089
  18 C Isotropic = 161.3419 Anisotropy = 40.1252

XX= 146.0298 YX= -3.1921 ZX= 11.5068
XY= -3.2960 YY= 168.7642 ZY= -15.0856
XZ= 13.2411 YZ= -17.0857 ZZ= 169.2318
Eigenvalues: 140.1175 155.8162 188.0920
19 H Isotropic = 29.6694 Anisotropy = 11.4078
XX= 34.6860 YX= 0.8145 ZX= -4.7205
XY= 0.1711 YY= 27.4843 ZY= -0.9676
XZ= -5.3969 YZ= -1.7286 ZZ= 26.8378
Eigenvalues: 24.0638 27.6697 37.2746
20 H Isotropic = 29.4007 Anisotropy = 3.2361
XX= 27.8608 YX= 0.6949 ZX= -1.1793
XY= 0.0687 YY= 29.3203 ZY= 0.6432
XZ= 0.4888 YZ= 1.5353 ZZ= 31.0209
Eigenvalues: 27.6423 29.0016 31.5581
21 H Isotropic = 29.8695 Anisotropy = 8.0823
XX= 30.1613 YX= 2.5660 ZX= -2.1309
XY= 1.9988 YY= 32.9665 ZY= -2.7021
XZ= -1.0592 YZ= -2.3512 ZZ= 26.4806
Eigenvalues: 25.4596 28.8911 35.2576
22 H Isotropic = 30.7455 Anisotropy = 8.2706
XX= 33.0782 YX= 1.5150 ZX= 2.9995
XY= 1.8092 YY= 29.3100 ZY= 2.6244
XZ= 3.5069 YZ= 2.6371 ZZ= 29.8481
Eigenvalues: 26.7161 29.2610 36.2592
23 H Isotropic = 28.7117 Anisotropy = 9.0405
XX= 31.2395 YX= -4.5385 ZX= 4.2819
XY= -2.2800 YY= 28.9773 ZY= -0.5245
XZ= 1.1757 YZ= -2.2399 ZZ= 25.9184
Eigenvalues: 24.7667 26.6298 34.7387
24 H Isotropic = 26.2121 Anisotropy = 4.5788
XX= 27.1291 YX= -0.2599 ZX= 0.5683
XY= 1.0520 YY= 28.0473 ZY= -2.2520
XZ= -0.1859 YZ= -2.9648 ZZ= 23.4598
Eigenvalues: 22.2566 27.1150 29.2646
25 H Isotropic = 27.7373 Anisotropy = 3.9187
XX= 27.6735 YX= -0.8279 ZX= -1.3662
XY= -2.1830 YY= 26.4837 ZY= -2.9640
XZ= 0.3774 YZ= -1.4050 ZZ= 29.0547
Eigenvalues: 24.4767 28.3855 30.3498
26 H Isotropic = 28.9314 Anisotropy = 6.7647
XX= 27.8541 YX= 1.8545 ZX= 0.6533
XY= 3.3261 YY= 31.0109 ZY= -2.2346
XZ= -2.4802 YZ= -2.0537 ZZ= 27.9292
Eigenvalues: 26.3127 27.0403 33.4412
27 H Isotropic = 29.7427 Anisotropy = 9.3362
XX= 32.3801 YX= 2.2462 ZX= 1.9592
XY= 2.2207 YY= 31.2481 ZY= 4.6953
XZ= 1.5991 YZ= 4.3254 ZZ= 25.5999

Eigenvalues: 23.0761 30.1851 35.9669
28 H Isotropic = 30.1977 Anisotropy = 6.2948
XX= 30.0383 YX= 0.2409 ZX= -0.4235
XY= -0.6829 YY= 30.3011 ZY= -3.8367
XZ= 1.3160 YZ= -4.2947 ZZ= 30.2536
Eigenvalues: 26.2048 29.9940 34.3942
29 H Isotropic = 29.1817 Anisotropy = 4.1120
XX= 28.0839 YX= 1.4744 ZX= -0.9544
XY= 2.1965 YY= 28.9326 ZY= 0.1235
XZ= -1.5729 YZ= -1.7909 ZZ= 30.5286
Eigenvalues: 26.5599 29.0621 31.9230
30 H Isotropic = 29.5282 Anisotropy = 9.7723
XX= 29.2394 YX= -3.3322 ZX= -1.7270
XY= -2.0514 YY= 31.8956 ZY= 4.0284
XZ= -0.7287 YZ= 5.1599 ZZ= 27.4496
Eigenvalues: 24.5297 28.0119 36.0430
31 H Isotropic = 26.2218 Anisotropy = 7.7247
XX= 28.3122 YX= 4.6626 ZX= 2.8759
XY= 2.2107 YY= 25.8845 ZY= 0.7564
XZ= 1.6119 YZ= 0.0511 ZZ= 24.4687
Eigenvalues: 22.6999 24.5939 31.3716
32 H Isotropic = 25.1995 Anisotropy = 5.3822
XX= 25.3359 YX= 1.7922 ZX= 1.2356
XY= 2.8149 YY= 26.0474 ZY= 0.8739
XZ= 2.5063 YZ= 0.7669 ZZ= 24.2153
Eigenvalues: 22.5828 24.2281 28.7877
33 H Isotropic = 30.6883 Anisotropy = 7.8818
XX= 35.7942 YX= 0.6112 ZX= 1.0467
XY= 1.4087 YY= 28.0045 ZY= -3.1228
XZ= 0.5314 YZ= -3.7199 ZZ= 28.2664
Eigenvalues: 24.5668 31.5554 35.9429
34 H Isotropic = 30.4617 Anisotropy = 6.5320
XX= 27.8143 YX= -0.8357 ZX= 1.2788
XY= -0.4730 YY= 29.0040 ZY= 0.7196
XZ= -0.6928 YZ= 1.6719 ZZ= 34.5668
Eigenvalues: 27.4394 29.1293 34.8164
35 H Isotropic = 30.3647 Anisotropy = 10.5030
XX= 27.2441 YX= -0.9000 ZX= 1.6313
XY= 0.1715 YY= 34.8876 ZY= -4.0958
XZ= 0.1435 YZ= -4.9030 ZZ= 28.9623
Eigenvalues: 26.1748 27.5525 37.3667
36 H Isotropic = 29.9710 Anisotropy = 7.5106
XX= 31.1789 YX= 0.4391 ZX= 3.5540
XY= -0.5291 YY= 28.7518 ZY= -2.1801
XZ= 4.8656 YZ= -0.5910 ZZ= 29.9821
Eigenvalues: 25.9462 28.9887 34.9780
37 H Isotropic = 30.1687 Anisotropy = 9.2050
XX= 27.8080 YX= -3.0576 ZX= 1.5641

XY= -2.0025 YY= 35.4601 ZY= 0.0618
XZ= 1.0648 YZ= -1.0845 ZZ= 27.2380
Eigenvalues: 25.9927 28.2081 36.3053
38 H Isotropic = 29.7475 Anisotropy = 5.3503
XX= 30.4499 YX= -0.3922 ZX= -1.1090
XY= -0.3702 YY= 27.1418 ZY= -2.3152
XZ= -1.6957 YZ= -2.9496 ZZ= 31.6506
Eigenvalues: 25.7387 30.1893 33.3143

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1 C Isotropic = 161.0097 Anisotropy = 16.4165
XX= 165.0185 YX= 3.8788 ZX= 7.4909
XY= 5.0440 YY= 168.9401 ZY= -4.6827
XZ= 3.6544 YZ= -5.7447 ZZ= 149.0706
Eigenvalues: 145.5847 165.4904 171.9541
2 C Isotropic = 154.9418 Anisotropy = 32.4425
XX= 149.1283 YX= 14.2308 ZX= -11.3480
XY= 7.7106 YY= 168.6835 ZY= -4.4534
XZ= -17.9358 YZ= -1.2889 ZZ= 147.0136
Eigenvalues: 132.5133 155.7419 176.5701
3 C Isotropic = 124.9053 Anisotropy = 66.9903
XX= 79.9524 YX= 24.2506 ZX= -3.1931
XY= 25.8699 YY= 149.0255 ZY= -15.6232
XZ= -6.9745 YZ= -17.2282 ZZ= 145.7380
Eigenvalues: 71.8175 133.3329 169.5655
4 C Isotropic = 124.2538 Anisotropy = 55.8254
XX= 93.2271 YX= 20.8910 ZX= 10.3498
XY= 9.7853 YY= 148.0034 ZY= -24.1370
XZ= 7.0070 YZ= -13.7605 ZZ= 131.5311
Eigenvalues: 85.1360 126.1547 161.4708
5 C Isotropic = 38.1576 Anisotropy = 179.4296
XX= 111.1361 YX= 62.3538 ZX= 17.6069
XY= 57.3328 YY= 20.3108 ZY= 75.9131
XZ= 23.0827 YZ= 72.5405 ZZ= -16.9740
Eigenvalues: -77.4645 34.1601 157.7774
6 C Isotropic = 53.4584 Anisotropy = 123.1522
XX= 109.9483 YX= 20.6308 ZX= 14.7925
XY= 34.0009 YY= 63.5726 ZY= 62.6824
XZ= 13.5636 YZ= 62.4609 ZZ= -13.1458
Eigenvalues: -48.1866 73.0019 135.5599
7 C Isotropic = 109.7315 Anisotropy = 59.6966
XX= 126.9660 YX= 12.8230 ZX= 25.6193
XY= 8.4081 YY= 103.7951 ZY= 16.5754
XZ= 27.6897 YZ= 14.8712 ZZ= 98.4334
Eigenvalues: 79.2291 100.4362 149.5292
8 C Isotropic = 141.5974 Anisotropy = 24.9678

XX= 155.5819 YX= -8.0201 ZX= 4.9683
XY= -4.5106 YY= 141.9018 ZY= 7.9204
XZ= 5.4205 YZ= 5.0533 ZZ= 127.3085
Eigenvalues: 123.2531 143.2965 158.2426
9 C Isotropic = 159.8693 Anisotropy = 21.9411
XX= 169.0606 YX= 10.2773 ZX= 1.1344
XY= 13.0933 YY= 147.1114 ZY= 5.0224
XZ= -1.4257 YZ= 5.6164 ZZ= 163.4359
Eigenvalues: 140.9636 164.1477 174.4967
10 C Isotropic = 158.7045 Anisotropy = 20.6053
XX= 160.5746 YX= 15.6334 ZX= -0.2389
XY= 14.9691 YY= 151.7996 ZY= 3.8082
XZ= 4.7620 YZ= -4.1471 ZZ= 163.7393
Eigenvalues: 140.1739 163.4983 172.4414
11 O Isotropic = 90.7215 Anisotropy = 152.2976
XX= 43.5292 YX= -118.1724 ZX= -108.7490
XY= -99.2575 YY= 111.4280 ZY= -70.1653
XZ= -62.4820 YZ= -66.8236 ZZ= 117.2073
Eigenvalues: -93.4146 173.3258 192.2532
12 C Isotropic = 13.0829 Anisotropy = 75.4349
XX= 22.3013 YX= 47.7647 ZX= 50.8392
XY= 40.9957 YY= 15.4054 ZY= -44.7371
XZ= 33.2384 YZ= -45.1615 ZZ= 1.5420
Eigenvalues: -75.0881 50.9639 63.3728
13 C Isotropic = 37.4553 Anisotropy = 151.0594
XX= 22.9012 YX= -66.8131 ZX= -9.6767
XY= -71.0241 YY= 36.1382 ZY= -77.6507
XZ= -3.4251 YZ= -73.5228 ZZ= 53.3266
Eigenvalues: -68.8661 43.0705 138.1616
14 O Isotropic = 263.4887 Anisotropy = 166.8411
XX= 307.2611 YX= -42.3523 ZX= -70.5796
XY= -36.4816 YY= 317.7378 ZY= -94.7913
XZ= -38.6808 YZ= -118.7358 ZZ= 165.4670
Eigenvalues: 90.0124 325.7375 374.7160
15 O Isotropic = -63.6044 Anisotropy = 585.1822
XX= -310.3888 YX= -60.2667 ZX= 55.9484
XY= -39.6845 YY= 61.8128 ZY= -256.5776
XZ= 27.3530 YZ= -263.6732 ZZ= 57.7629
Eigenvalues: -317.2529 -200.0773 326.5171
16 C Isotropic = 61.7236 Anisotropy = 173.9234
XX= 31.3301 YX= -74.8598 ZX= -3.9097
XY= -81.7860 YY= 68.2782 ZY= -80.3776
XZ= 4.4606 YZ= -77.0000 ZZ= 85.5624
Eigenvalues: -51.1223 58.6205 177.6725
17 C Isotropic = 160.7197 Anisotropy = 43.7512
XX= 150.4393 YX= -9.8105 ZX= -12.8471
XY= -3.9492 YY= 182.1527 ZY= -16.8704
XZ= -9.1378 YZ= -18.1703 ZZ= 149.5672

Eigenvalues: 132.6530 159.6190 189.8872
18 C Isotropic = 160.0148 Anisotropy = 41.2801
XX= 145.0965 YX= -8.3104 ZX= 6.4524
XY= -11.2798 YY= 174.4359 ZY= -17.0855
XZ= 2.6172 YZ= -14.7404 ZZ= 160.5119
Eigenvalues: 142.1197 150.3897 187.5349
19 H Isotropic = 29.2003 Anisotropy = 3.8328
XX= 29.6791 YX= 0.0557 ZX= 2.6329
XY= 1.4285 YY= 28.3995 ZY= 1.1754
XZ= 0.5088 YZ= 1.2960 ZZ= 29.5222
Eigenvalues: 27.5547 28.2905 31.7555
20 H Isotropic = 29.8186 Anisotropy = 11.0283
XX= 36.4072 YX= 0.4187 ZX= -3.3090
XY= 1.7595 YY= 28.8220 ZY= -0.7175
XZ= -2.1266 YZ= -0.9582 ZZ= 24.2265
Eigenvalues: 23.5791 28.7058 37.1708
21 H Isotropic = 29.9283 Anisotropy = 8.5209
XX= 31.0014 YX= -2.6505 ZX= -3.1167
XY= -2.5954 YY= 32.9761 ZY= 0.1536
XZ= -4.6288 YZ= 0.8999 ZZ= 25.8074
Eigenvalues: 23.6726 30.5034 35.6089
22 H Isotropic = 29.9271 Anisotropy = 6.1249
XX= 28.1462 YX= 0.2932 ZX= -0.5508
XY= 0.3144 YY= 27.7367 ZY= 0.4075
XZ= -0.6602 YZ= 0.7673 ZZ= 33.8984
Eigenvalues: 27.4735 28.2975 34.0104
23 H Isotropic = 29.3397 Anisotropy = 8.7816
XX= 31.3314 YX= 1.4161 ZX= 1.1093
XY= 4.5389 YY= 31.7173 ZY= -3.8339
XZ= -0.2020 YZ= -3.7986 ZZ= 24.9706
Eigenvalues: 22.9076 29.9175 35.1941
24 H Isotropic = 26.2870 Anisotropy = 4.7096
XX= 26.5272 YX= -1.3052 ZX= -2.3580
XY= -2.1483 YY= 28.3882 ZY= -0.5057
XZ= -1.4593 YZ= -1.3544 ZZ= 23.9455
Eigenvalues: 22.4646 26.9697 29.4267
25 H Isotropic = 27.0696 Anisotropy = 4.9436
XX= 29.7058 YX= 1.8010 ZX= -0.9567
XY= 1.4205 YY= 25.8347 ZY= -0.3396
XZ= -0.3890 YZ= 0.5322 ZZ= 25.6683
Eigenvalues: 25.0622 25.7812 30.3653
26 H Isotropic = 28.6748 Anisotropy = 6.5017
XX= 27.6163 YX= -0.3683 ZX= 1.2555
XY= 2.2222 YY= 30.7867 ZY= -3.3211
XZ= -0.1918 YZ= -3.4974 ZZ= 27.6214
Eigenvalues: 25.0864 27.9287 33.0093
27 H Isotropic = 29.7385 Anisotropy = 4.6029
XX= 29.4124 YX= 0.6591 ZX= -1.8231

XY= -1.2542 YY= 27.9927 ZY= -1.6740
XZ= -0.8723 YZ= -1.5360 ZZ= 31.8104
Eigenvalues: 27.1356 29.2728 32.8071
28 H Isotropic = 29.5153 Anisotropy = 8.6012
XX= 31.6228 YX= -2.3405 ZX= -2.1803
XY= -1.1478 YY= 30.8534 ZY= 4.0635
XZ= -2.4752 YZ= 4.1552 ZZ= 26.0698
Eigenvalues: 23.5276 29.7689 35.2495
29 H Isotropic = 29.9242 Anisotropy = 9.7819
XX= 28.1251 YX= 3.6311 ZX= 2.0463
XY= 1.9893 YY= 32.2019 ZY= 4.2113
XZ= 0.3900 YZ= 4.4469 ZZ= 29.4457
Eigenvalues: 25.9191 27.4081 36.4455
30 H Isotropic = 28.3050 Anisotropy = 4.6200
XX= 28.6549 YX= -2.2681 ZX= 0.9014
XY= -1.8869 YY= 29.4416 ZY= 1.3140
XZ= 2.0486 YZ= -1.4071 ZZ= 26.8184
Eigenvalues: 25.6736 27.8563 31.3850
31 H Isotropic = 26.1949 Anisotropy = 8.1323
XX= 29.7293 YX= -2.3463 ZX= -3.9985
XY= -0.8640 YY= 23.4672 ZY= -0.7436
XZ= -2.2965 YZ= 0.5415 ZZ= 25.3880
Eigenvalues: 22.6235 24.3447 31.6164
32 H Isotropic = 25.1978 Anisotropy = 5.3801
XX= 26.7050 YX= -1.1371 ZX= -1.5575
XY= -2.5617 YY= 23.4033 ZY= 0.8203
XZ= -2.3165 YZ= 0.4615 ZZ= 25.4849
Eigenvalues: 22.5548 24.2540 28.7845
33 H Isotropic = 30.2488 Anisotropy = 10.1414
XX= 26.6194 YX= -1.0368 ZX= -1.2726
XY= -1.7078 YY= 35.5844 ZY= 3.9099
XZ= -0.0638 YZ= 2.3883 ZZ= 28.5427
Eigenvalues: 26.3785 27.3582 37.0097
34 H Isotropic = 30.1961 Anisotropy = 9.1032
XX= 31.8408 YX= -2.1409 ZX= 2.4622
XY= -4.0891 YY= 30.7859 ZY= -2.5941
XZ= 3.4266 YZ= -2.3906 ZZ= 27.9615
Eigenvalues: 26.1693 28.1541 36.2649
35 H Isotropic = 31.1998 Anisotropy = 10.7576
XX= 29.8762 YX= 1.2752 ZX= -2.8932
XY= 1.6571 YY= 34.1376 ZY= -5.1834
XZ= -2.6699 YZ= -5.0548 ZZ= 29.5856
Eigenvalues: 25.6113 29.6166 38.3716
36 H Isotropic = 29.9990 Anisotropy = 7.1552
XX= 26.8566 YX= -0.6522 ZX= -0.2805
XY= -0.0669 YY= 29.8591 ZY= -3.6029
XZ= -1.8738 YZ= -1.6190 ZZ= 33.2812
Eigenvalues: 26.4416 28.7862 34.7691

37 H Isotropic = 29.9619 Anisotropy = 5.2120
XX= 32.0461 YX= -1.4590 ZX= -0.8531
XY= -1.7039 YY= 30.8806 ZY= -2.1638
XZ= 0.0185 YZ= -3.1722 ZZ= 26.9590
Eigenvalues: 25.4244 31.0247 33.4366
38 H Isotropic = 29.9408 Anisotropy = 9.8641
XX= 27.2591 YX= 2.9586 ZX= 0.1987
XY= 2.3966 YY= 35.6772 ZY= 1.1317
XZ= 0.3923 YZ= 0.2813 ZZ= 26.8859
Eigenvalues: 26.4595 26.8460 36.5169

RSSRZ

1 C Isotropic = 161.0097 Anisotropy = 16.4165
XX= 165.0185 YX= 3.8788 ZX= 7.4909
XY= 5.0440 YY= 168.9401 ZY= -4.6827
XZ= 3.6544 YZ= -5.7447 ZZ= 149.0706
Eigenvalues: 145.5847 165.4904 171.9541
2 C Isotropic = 154.9418 Anisotropy = 32.4425
XX= 149.1283 YX= 14.2308 ZX= -11.3480
XY= 7.7106 YY= 168.6835 ZY= -4.4534
XZ= -17.9358 YZ= -1.2889 ZZ= 147.0136
Eigenvalues: 132.5133 155.7419 176.5701
3 C Isotropic = 124.9053 Anisotropy = 66.9903
XX= 79.9524 YX= 24.2506 ZX= -3.1931
XY= 25.8699 YY= 149.0255 ZY= -15.6232
XZ= -6.9745 YZ= -17.2282 ZZ= 145.7380
Eigenvalues: 71.8175 133.3329 169.5655
4 C Isotropic = 124.2538 Anisotropy = 55.8254
XX= 93.2271 YX= 20.8910 ZX= 10.3498
XY= 9.7853 YY= 148.0034 ZY= -24.1370
XZ= 7.0070 YZ= -13.7605 ZZ= 131.5311
Eigenvalues: 85.1360 126.1547 161.4708
5 C Isotropic = 38.1576 Anisotropy = 179.4296
XX= 111.1361 YX= 62.3538 ZX= 17.6069
XY= 57.3328 YY= 20.3108 ZY= 75.9131
XZ= 23.0827 YZ= 72.5405 ZZ= -16.9740
Eigenvalues: -77.4645 34.1601 157.7774
6 C Isotropic = 53.4584 Anisotropy = 123.1522
XX= 109.9483 YX= 20.6308 ZX= 14.7925
XY= 34.0009 YY= 63.5726 ZY= 62.6824
XZ= 13.5636 YZ= 62.4609 ZZ= -13.1458
Eigenvalues: -48.1866 73.0019 135.5599
7 C Isotropic = 109.7315 Anisotropy = 59.6966
XX= 126.9660 YX= 12.8230 ZX= 25.6193
XY= 8.4081 YY= 103.7951 ZY= 16.5754
XZ= 27.6897 YZ= 14.8712 ZZ= 98.4334

Eigenvalues: 79.2291 100.4362 149.5292
  8 C Isotropic = 141.5974 Anisotropy = 24.9678
XX= 155.5819 YX= -8.0201 ZX= 4.9683
XY= -4.5106 YY= 141.9018 ZY= 7.9204
XZ= 5.4205 YZ= 5.0533 ZZ= 127.3085
Eigenvalues: 123.2531 143.2965 158.2426
  9 C Isotropic = 159.8693 Anisotropy = 21.9411
XX= 169.0606 YX= 10.2773 ZX= 1.1344
XY= 13.0933 YY= 147.1114 ZY= 5.0224
XZ= -1.4257 YZ= 5.6164 ZZ= 163.4359
Eigenvalues: 140.9636 164.1477 174.4967
  10 C Isotropic = 158.7045 Anisotropy = 20.6053
XX= 160.5746 YX= 15.6334 ZX= -0.2389
XY= 14.9691 YY= 151.7996 ZY= 3.8082
XZ= 4.7620 YZ= -4.1471 ZZ= 163.7393
Eigenvalues: 140.1739 163.4983 172.4414
  11 O Isotropic = 90.7215 Anisotropy = 152.2976
XX= 43.5292 YX= -118.1724 ZX= -108.7490
XY= -99.2575 YY= 111.4280 ZY= -70.1653
XZ= -62.4820 YZ= -66.8236 ZZ= 117.2073
Eigenvalues: -93.4146 173.3258 192.2532
  12 C Isotropic = 13.0829 Anisotropy = 75.4349
XX= 22.3013 YX= 47.7647 ZX= 50.8392
XY= 40.9957 YY= 15.4054 ZY= -44.7371
XZ= 33.2384 YZ= -45.1615 ZZ= 1.5420
Eigenvalues: -75.0881 50.9639 63.3728
  13 C Isotropic = 37.4553 Anisotropy = 151.0594
XX= 22.9012 YX= -66.8131 ZX= -9.6767
XY= -71.0241 YY= 36.1382 ZY= -77.6507
XZ= -3.4251 YZ= -73.5228 ZZ= 53.3266
Eigenvalues: -68.8661 43.0705 138.1616
  14 O Isotropic = 263.4887 Anisotropy = 166.8411
XX= 307.2611 YX= -42.3523 ZX= -70.5796
XY= -36.4816 YY= 317.7378 ZY= -94.7913
XZ= -38.6808 YZ= -118.7358 ZZ= 165.4670
Eigenvalues: 90.0124 325.7375 374.7160
  15 O Isotropic = -63.6044 Anisotropy = 585.1822
XX= -310.3888 YX= -60.2667 ZX= 55.9484
XY= -39.6845 YY= 61.8128 ZY= -256.5776
XZ= 27.3530 YZ= -263.6732 ZZ= 57.7629
Eigenvalues: -317.2529 -200.0773 326.5171
  16 C Isotropic = 61.7236 Anisotropy = 173.9234
XX= 31.3301 YX= -74.8598 ZX= -3.9097
XY= -81.7860 YY= 68.2782 ZY= -80.3776
XZ= 4.4606 YZ= -77.0000 ZZ= 85.5624
Eigenvalues: -51.1223 58.6205 177.6725
  17 C Isotropic = 160.7197 Anisotropy = 43.7512
XX= 150.4393 YX= -9.8105 ZX= -12.8471

XY= -3.9492 YY= 182.1527 ZY= -16.8704
XZ= -9.1378 YZ= -18.1703 ZZ= 149.5672
Eigenvalues: 132.6530 159.6190 189.8872
 18 C Isotropic = 160.0148 Anisotropy = 41.2801
XX= 145.0965 YX= -8.3104 ZX= 6.4524
XY= -11.2798 YY= 174.4359 ZY= -17.0855
XZ= 2.6172 YZ= -14.7404 ZZ= 160.5119
Eigenvalues: 142.1197 150.3897 187.5349
 19 H Isotropic = 29.2003 Anisotropy = 3.8328
XX= 29.6791 YX= 0.0557 ZX= 2.6329
XY= 1.4285 YY= 28.3995 ZY= 1.1754
XZ= 0.5088 YZ= 1.2960 ZZ= 29.5222
Eigenvalues: 27.5547 28.2905 31.7555
 20 H Isotropic = 29.8186 Anisotropy = 11.0283
XX= 36.4072 YX= 0.4187 ZX= -3.3090
XY= 1.7595 YY= 28.8220 ZY= -0.7175
XZ= -2.1266 YZ= -0.9582 ZZ= 24.2265
Eigenvalues: 23.5791 28.7058 37.1708
 21 H Isotropic = 29.9283 Anisotropy = 8.5209
XX= 31.0014 YX= -2.6505 ZX= -3.1167
XY= -2.5954 YY= 32.9761 ZY= 0.1536
XZ= -4.6288 YZ= 0.8999 ZZ= 25.8074
Eigenvalues: 23.6726 30.5034 35.6089
 22 H Isotropic = 29.9271 Anisotropy = 6.1249
XX= 28.1462 YX= 0.2932 ZX= -0.5508
XY= 0.3144 YY= 27.7367 ZY= 0.4075
XZ= -0.6602 YZ= 0.7673 ZZ= 33.8984
Eigenvalues: 27.4735 28.2975 34.0104
 23 H Isotropic = 29.3397 Anisotropy = 8.7816
XX= 31.3314 YX= 1.4161 ZX= 1.1093
XY= 4.5389 YY= 31.7173 ZY= -3.8339
XZ= -0.2020 YZ= -3.7986 ZZ= 24.9706
Eigenvalues: 22.9076 29.9175 35.1941
 24 H Isotropic = 26.2870 Anisotropy = 4.7096
XX= 26.5272 YX= -1.3052 ZX= -2.3580
XY= -2.1483 YY= 28.3882 ZY= -0.5057
XZ= -1.4593 YZ= -1.3544 ZZ= 23.9455
Eigenvalues: 22.4646 26.9697 29.4267
 25 H Isotropic = 27.0696 Anisotropy = 4.9436
XX= 29.7058 YX= 1.8010 ZX= -0.9567
XY= 1.4205 YY= 25.8347 ZY= -0.3396
XZ= -0.3890 YZ= 0.5322 ZZ= 25.6683
Eigenvalues: 25.0622 25.7812 30.3653
 26 H Isotropic = 28.6748 Anisotropy = 6.5017
XX= 27.6163 YX= -0.3683 ZX= 1.2555
XY= 2.2222 YY= 30.7867 ZY= -3.3211
XZ= -0.1918 YZ= -3.4974 ZZ= 27.6214
Eigenvalues: 25.0864 27.9287 33.0093

27 H Isotropic = 29.7385 Anisotropy = 4.6029
XX= 29.4124 YX= 0.6591 ZX= -1.8231
XY= -1.2542 YY= 27.9927 ZY= -1.6740
XZ= -0.8723 YZ= -1.5360 ZZ= 31.8104
Eigenvalues: 27.1356 29.2728 32.8071
28 H Isotropic = 29.5153 Anisotropy = 8.6012
XX= 31.6228 YX= -2.3405 ZX= -2.1803
XY= -1.1478 YY= 30.8534 ZY= 4.0635
XZ= -2.4752 YZ= 4.1552 ZZ= 26.0698
Eigenvalues: 23.5276 29.7689 35.2495
29 H Isotropic = 29.9242 Anisotropy = 9.7819
XX= 28.1251 YX= 3.6311 ZX= 2.0463
XY= 1.9893 YY= 32.2019 ZY= 4.2113
XZ= 0.3900 YZ= 4.4469 ZZ= 29.4457
Eigenvalues: 25.9191 27.4081 36.4455
30 H Isotropic = 28.3050 Anisotropy = 4.6200
XX= 28.6549 YX= -2.2681 ZX= 0.9014
XY= -1.8869 YY= 29.4416 ZY= 1.3140
XZ= 2.0486 YZ= -1.4071 ZZ= 26.8184
Eigenvalues: 25.6736 27.8563 31.3850
31 H Isotropic = 26.1949 Anisotropy = 8.1323
XX= 29.7293 YX= -2.3463 ZX= -3.9985
XY= -0.8640 YY= 23.4672 ZY= -0.7436
XZ= -2.2965 YZ= 0.5415 ZZ= 25.3880
Eigenvalues: 22.6235 24.3447 31.6164
32 H Isotropic = 25.1978 Anisotropy = 5.3801
XX= 26.7050 YX= -1.1371 ZX= -1.5575
XY= -2.5617 YY= 23.4033 ZY= 0.8203
XZ= -2.3165 YZ= 0.4615 ZZ= 25.4849
Eigenvalues: 22.5548 24.2540 28.7845
33 H Isotropic = 30.2488 Anisotropy = 10.1414
XX= 26.6194 YX= -1.0368 ZX= -1.2726
XY= -1.7078 YY= 35.5844 ZY= 3.9099
XZ= -0.0638 YZ= 2.3883 ZZ= 28.5427
Eigenvalues: 26.3785 27.3582 37.0097
34 H Isotropic = 30.1961 Anisotropy = 9.1032
XX= 31.8408 YX= -2.1409 ZX= 2.4622
XY= -4.0891 YY= 30.7859 ZY= -2.5941
XZ= 3.4266 YZ= -2.3906 ZZ= 27.9615
Eigenvalues: 26.1693 28.1541 36.2649
35 H Isotropic = 31.1998 Anisotropy = 10.7576
XX= 29.8762 YX= 1.2752 ZX= -2.8932
XY= 1.6571 YY= 34.1376 ZY= -5.1834
XZ= -2.6699 YZ= -5.0548 ZZ= 29.5856
Eigenvalues: 25.6113 29.6166 38.3716
36 H Isotropic = 29.9990 Anisotropy = 7.1552
XX= 26.8566 YX= -0.6522 ZX= -0.2805
XY= -0.0669 YY= 29.8591 ZY= -3.6029

XZ= -1.8738 YZ= -1.6190 ZZ= 33.2812
Eigenvalues: 26.4416 28.7862 34.7691
37 H Isotropic = 29.9619 Anisotropy = 5.2120
XX= 32.0461 YX= -1.4590 ZX= -0.8531
XY= -1.7039 YY= 30.8806 ZY= -2.1638
XZ= 0.0185 YZ= -3.1722 ZZ= 26.9590
Eigenvalues: 25.4244 31.0247 33.4366
38 H Isotropic = 29.9408 Anisotropy = 9.8641
XX= 27.2591 YX= 2.9586 ZX= 0.1987
XY= 2.3966 YY= 35.6772 ZY= 1.1317
XZ= 0.3923 YZ= 0.2813 ZZ= 26.8859
Eigenvalues: 26.4595 26.8460 36.5169

RSRSZ

1 C Isotropic = 161.4420 Anisotropy = 16.3088
XX= 165.5388 YX= -3.1338 ZX= -5.5939
XY= -0.4434 YY= 171.6544 ZY= -3.0930
XZ= -6.1944 YZ= -3.9018 ZZ= 147.1327
Eigenvalues: 144.8509 167.1605 172.3145
2 C Isotropic = 150.4973 Anisotropy = 23.2233
XX= 147.8242 YX= -13.1144 ZX= 9.0112
XY= -6.8333 YY= 150.5636 ZY= -6.0535
XZ= 8.7685 YZ= -2.5837 ZZ= 153.1041
Eigenvalues: 137.8209 147.6915 165.9795
3 C Isotropic = 123.7372 Anisotropy = 53.4299
XX= 82.8876 YX= -18.1020 ZX= -4.5859
XY= -21.5573 YY= 135.9604 ZY= -13.6363
XZ= -1.1663 YZ= -10.2777 ZZ= 152.3635
Eigenvalues: 75.7336 136.1208 159.3571
4 C Isotropic = 123.2843 Anisotropy = 49.0934
XX= 93.1941 YX= -12.3958 ZX= -11.0166
XY= -3.4707 YY= 129.3789 ZY= -9.3121
XZ= -10.7102 YZ= -19.9424 ZZ= 147.2798
Eigenvalues: 88.1930 125.6466 156.0132
5 C Isotropic = 39.1918 Anisotropy = 175.8491
XX= 111.2980 YX= -51.2282 ZX= -31.2249
XY= -45.4678 YY= -0.3511 ZY= 82.4587
XZ= -33.4376 YZ= 78.8561 ZZ= 6.6284
Eigenvalues: -78.5218 39.6727 156.4245
6 C Isotropic = 53.3395 Anisotropy = 123.4760
XX= 109.4018 YX= -18.6896 ZX= -20.5162
XY= -27.7736 YY= 46.8415 ZY= 71.8923
XZ= -20.9735 YZ= 68.9710 ZZ= 3.7751
Eigenvalues: -48.3955 72.7572 135.6568
7 C Isotropic = 106.5250 Anisotropy = 54.8849
XX= 128.6336 YX= -10.1249 ZX= -17.6725

XY= -16.7063 YY= 106.2100 ZY=   9.2197
XZ= -23.0898 YZ=   6.9409 ZZ=   84.7314
Eigenvalues: 76.4627   99.9974 143.1149
  8 C   Isotropic = 145.9573 Anisotropy =   26.1712
XX= 161.1387 YX=   7.4662 ZX=   -3.4295
XY=   4.4671 YY= 146.5932 ZY=   6.2671
XZ=   -4.6417 YZ=   4.2676 ZZ= 130.1400
Eigenvalues: 127.6495 146.8177 163.4048
  9 C   Isotropic = 158.7201 Anisotropy =   26.2104
XX= 172.8004 YX=   -6.8107 ZX=   -2.7956
XY= -12.0056 YY= 140.7749 ZY=   5.2217
XZ=   -0.5651 YZ=   7.3021 ZZ= 162.5850
Eigenvalues: 136.9770 162.9896 176.1937
  10 C   Isotropic = 156.9221 Anisotropy =   14.0879
XX= 158.8880 YX= -12.4067 ZX=   -0.6605
XY=   -8.6601 YY= 148.4351 ZY=   0.1710
XZ=   -0.7385 YZ=   -7.8967 ZZ= 163.4431
Eigenvalues: 141.2984 163.1539 166.3140
  11 O   Isotropic =   86.2403 Anisotropy = 161.8085
XX=   15.2420 YX= 141.5103 ZX=   87.1903
XY= 108.3091 YY= 106.6900 ZY= -43.1178
XZ=   52.2620 YZ= -49.4135 ZZ= 136.7888
Eigenvalues: -101.4284 166.0366 194.1126
  12 C   Isotropic =   13.8742 Anisotropy =   74.5244
XX=   36.1640 YX= -49.2691 ZX= -36.5245
XY= -39.7055 YY=   -8.6942 ZY= -49.0438
XZ= -23.4299 YZ= -47.9146 ZZ=   14.1528
Eigenvalues: -73.2554   51.3209   63.5572
  13 C   Isotropic =   37.1325 Anisotropy = 146.5362
XX=   9.0238 YX=   65.4262 ZX=   6.2472
XY=   65.3210 YY=   23.1696 ZY= -70.7771
XZ=   2.1644 YZ= -64.8900 ZZ=   79.2040
Eigenvalues: -67.5045   44.0787 134.8233
  14 O   Isotropic = 258.0939 Anisotropy = 141.6595
XX= 320.0771 YX=   29.0651 ZX=   4.2146
XY=   40.5339 YY= 136.9705 ZY= -90.4032
XZ=   3.2781 YZ= -75.3023 ZZ= 317.2340
Eigenvalues: 99.4933 322.2547 352.5335
  15 O   Isotropic = -59.9871 Anisotropy = 583.2668
XX= -309.5461 YX=   31.0042 ZX= -58.5877
XY=   20.5616 YY= -14.8706 ZY= -247.1701
XZ= -34.5885 YZ= -247.1713 ZZ= 144.4555
Eigenvalues: -314.2802 -194.5384 328.8574
  16 C   Isotropic =   61.4675 Anisotropy = 173.0254
XX=   14.2629 YX=   70.2147 ZX=   0.5901
XY=   75.2720 YY=   58.9526 ZY= -73.7852
XZ=   -6.4540 YZ= -73.1851 ZZ= 111.1871
Eigenvalues: -51.6540   59.2388 176.8178

17 C Isotropic = 164.4207 Anisotropy = 38.8979
XX= 164.6722 YX= 4.5004 ZX= -9.6203
XY= 10.3418 YY= 149.5902 ZY= -16.1437
XZ= -7.7073 YZ= -14.9351 ZZ= 178.9997
Eigenvalues: 142.3150 160.5944 190.3526
18 C Isotropic = 162.5793 Anisotropy = 38.3397
XX= 148.2483 YX= 6.8013 ZX= -4.7925
XY= 7.6308 YY= 181.9835 ZY= -12.2297
XZ= -2.1692 YZ= -10.7684 ZZ= 157.5062
Eigenvalues: 146.5968 153.0019 188.1391
19 H Isotropic = 29.7457 Anisotropy = 10.7529
XX= 35.1109 YX= -0.0793 ZX= 5.2130
XY= -0.5957 YY= 28.5498 ZY= -0.6586
XZ= 3.6738 YZ= -1.2759 ZZ= 25.5764
Eigenvalues: 23.7015 28.6213 36.9143
20 H Isotropic = 29.4955 Anisotropy = 4.3824
XX= 30.2086 YX= 0.3250 ZX= -3.4417
XY= -1.3733 YY= 28.8023 ZY= 0.1233
XZ= -1.5250 YZ= 0.1409 ZZ= 29.4756
Eigenvalues: 27.2917 28.7777 32.4171
21 H Isotropic = 29.7992 Anisotropy = 8.7789
XX= 30.0977 YX= 2.5395 ZX= 2.9561
XY= 2.7641 YY= 32.2890 ZY= 1.4112
XZ= 4.5127 YZ= 2.1930 ZZ= 27.0109
Eigenvalues: 24.5135 29.2323 35.6518
22 H Isotropic = 30.3364 Anisotropy = 5.5358
XX= 29.2246 YX= -0.4857 ZX= 0.0059
XY= -0.8978 YY= 27.7738 ZY= 0.0974
XZ= 0.4825 YZ= 0.2744 ZZ= 34.0108
Eigenvalues: 27.4861 29.4961 34.0269
23 H Isotropic = 29.2467 Anisotropy = 5.6965
XX= 26.7501 YX= 3.4553 ZX= 1.1664
XY= 2.8320 YY= 29.0929 ZY= -2.6158
XZ= 4.1402 YZ= -0.5571 ZZ= 31.8972
Eigenvalues: 23.4410 31.2548 33.0444
24 H Isotropic = 25.9950 Anisotropy = 4.6950
XX= 26.3651 YX= 1.3234 ZX= 2.5991
XY= 2.1818 YY= 27.6829 ZY= 0.1786
XZ= 1.8620 YZ= -0.9002 ZZ= 23.9370
Eigenvalues: 22.3229 26.5372 29.1250
25 H Isotropic = 27.4163 Anisotropy = 4.3699
XX= 29.9926 YX= -0.9299 ZX= 0.9135
XY= -1.3021 YY= 25.4300 ZY= -0.6205
XZ= -0.1267 YZ= -0.6006 ZZ= 26.8263
Eigenvalues: 25.0253 26.8941 30.3296
26 H Isotropic = 28.5834 Anisotropy = 6.4171
XX= 27.6287 YX= 0.1695 ZX= -0.8280
XY= -2.0618 YY= 30.2358 ZY= -3.3796

XZ= 0.4407 YZ= -3.6750 ZZ= 27.8857
Eigenvalues: 25.1358 27.7530 32.8615
 27 H Isotropic = 29.3658 Anisotropy = 7.9837
XX= 30.5794 YX= 2.3265 ZX= 1.3921
XY= 1.3500 YY= 31.5888 ZY= 3.4148
XZ= 1.7689 YZ= 3.7873 ZZ= 25.9293
Eigenvalues: 24.1141 29.2951 34.6883
 28 H Isotropic = 30.0073 Anisotropy = 5.5856
XX= 29.9577 YX= -1.0085 ZX= 2.3799
XY= 0.7601 YY= 27.6325 ZY= -1.3393
XZ= 1.5284 YZ= -1.1789 ZZ= 32.4316
Eigenvalues: 27.2626 29.0282 33.7310
 29 H Isotropic = 29.7568 Anisotropy = 9.4693
XX= 29.1842 YX= -2.7673 ZX= -3.5082
XY= -1.7699 YY= 29.2080 ZY= 4.1425
XZ= -1.8738 YZ= 4.1462 ZZ= 30.8783
Eigenvalues: 25.8141 27.3867 36.0697
 30 H Isotropic = 28.9355 Anisotropy = 7.3163
XX= 29.1752 YX= 2.9921 ZX= 0.6227
XY= 2.9449 YY= 31.9125 ZY= 0.9783
XZ= -0.8457 YZ= -0.7018 ZZ= 25.7189
Eigenvalues: 25.7005 27.2931 33.8130
 31 H Isotropic = 26.2237 Anisotropy = 8.2016
XX= 29.4000 YX= 3.6716 ZX= 3.5474
XY= 1.8578 YY= 24.0719 ZY= -0.1003
XZ= 1.9537 YZ= 0.8572 ZZ= 25.1992
Eigenvalues: 22.5874 24.3923 31.6915
 32 H Isotropic = 25.1607 Anisotropy = 5.2401
XX= 26.1580 YX= 1.5143 ZX= 1.1957
XY= 3.0723 YY= 24.1420 ZY= 1.1720
XZ= 1.8923 YZ= 0.9117 ZZ= 25.1822
Eigenvalues: 22.6445 24.1836 28.6541
 33 H Isotropic = 30.3908 Anisotropy = 10.3956
XX= 30.9287 YX= 4.9410 ZX= -0.4230
XY= 5.3277 YY= 32.1577 ZY= -1.5956
XZ= -2.2933 YZ= -2.3222 ZZ= 28.0860
Eigenvalues: 26.3070 27.5442 37.3212
 34 H Isotropic = 31.0916 Anisotropy = 9.9304
XX= 29.5296 YX= -0.2674 ZX= 1.6383
XY= 0.3091 YY= 28.8531 ZY= -4.6789
XZ= 1.7670 YZ= -4.6765 ZZ= 34.8922
Eigenvalues: 26.0912 29.4718 37.7119
 35 H Isotropic = 29.8729 Anisotropy = 7.2731
XX= 28.9881 YX= -1.9751 ZX= -3.5844
XY= -0.9782 YY= 29.3042 ZY= -0.1029
XZ= -4.5783 YZ= 1.1424 ZZ= 31.3264
Eigenvalues: 25.6921 29.2050 34.7216
 36 H Isotropic = 29.9322 Anisotropy = 7.6240

XX= 27.1850 YX= 0.3865 ZX= 1.2812
XY= -0.5680 YY= 30.5167 ZY= -4.1471
XZ= 2.7144 YZ= -2.3911 ZZ= 32.0949
Eigenvalues: 26.1281 28.6536 35.0148
37 H Isotropic = 30.0597 Anisotropy = 9.8391
XX= 27.0928 YX= -2.8646 ZX= -0.5980
XY= -2.0862 YY= 35.3058 ZY= 2.7387
XZ= -0.6133 YZ= 1.8032 ZZ= 27.7805
Eigenvalues: 26.4037 27.1563 36.6191
38 H Isotropic = 29.9193 Anisotropy = 5.0871
XX= 32.5567 YX= 1.0397 ZX= 0.5891
XY= 1.2099 YY= 30.8051 ZY= -2.3204
XZ= -0.0622 YZ= -3.2186 ZZ= 26.3961
Eigenvalues: 24.9901 31.4570 33.3107

RRSRZ

1 C Isotropic = 158.0913 Anisotropy = 16.1219
XX= 149.5623 YX= -7.6021 ZX= 5.3340
XY= -9.1268 YY= 162.4038 ZY= -2.5846
XZ= 0.6555 YZ= -3.0681 ZZ= 162.3078
Eigenvalues: 145.3118 160.1228 168.8392
2 C Isotropic = 146.3612 Anisotropy = 39.0203
XX= 149.0720 YX= -2.9553 ZX= 18.0230
XY= -3.3616 YY= 135.4259 ZY= 8.7651
XZ= 22.0465 YZ= 5.7417 ZZ= 154.5858
Eigenvalues: 126.0238 140.6852 172.3748
3 C Isotropic = 124.5508 Anisotropy = 55.7664
XX= 87.1479 YX= -14.4752 ZX= 22.0079
XY= -16.5827 YY= 131.9070 ZY= 3.5832
XZ= 23.6241 YZ= 1.9105 ZZ= 154.5974
Eigenvalues: 75.7862 136.1377 161.7284
4 C Isotropic = 124.0254 Anisotropy = 47.7132
XX= 100.3402 YX= -13.7354 ZX= 16.4203
XY= -3.3611 YY= 123.6448 ZY= 6.5728
XZ= 21.8267 YZ= 11.2512 ZZ= 148.0911
Eigenvalues: 89.9688 126.2732 155.8342
5 C Isotropic = 39.3450 Anisotropy = 173.1490
XX= -29.5158 YX= 29.1498 ZX= 53.9162
XY= 33.4217 YY= 51.6728 ZY= -75.1632
XZ= 51.5338 YZ= -73.6558 ZZ= 95.8781
Eigenvalues: -76.2234 39.4808 154.7777
6 C Isotropic = 57.0339 Anisotropy = 119.9486
XX= -16.8913 YX= 24.2798 ZX= 43.4175
XY= 21.8169 YY= 90.3976 ZY= -42.8448
XZ= 44.5984 YZ= -38.3743 ZZ= 97.5954
Eigenvalues: -41.5392 75.6414 136.9997
7 C Isotropic = 101.8208 Anisotropy = 46.5695

XX= 129.1656 YX= -1.2661 ZX= -9.4457
XY= -12.7964 YY= 92.3385 ZY= 9.0171
XZ= -9.0019 YZ= 9.0216 ZZ= 83.9582
Eigenvalues: 77.8524 94.7429 132.8671
8 C Isotropic = 139.4677 Anisotropy = 16.9391
XX= 149.1064 YX= 3.6402 ZX= -2.2040
XY= 1.9856 YY= 141.5777 ZY= -0.1522
XZ= -6.4991 YZ= 0.6702 ZZ= 127.7191
Eigenvalues: 126.8239 140.8188 150.7605
9 C Isotropic = 161.4368 Anisotropy = 23.8351
XX= 168.5819 YX= -4.4655 ZX= 9.9349
XY= -3.7274 YY= 150.1534 ZY= -0.8232
XZ= 8.2292 YZ= -5.9759 ZZ= 165.5749
Eigenvalues: 149.1103 157.8731 177.3268
10 C Isotropic = 156.9552 Anisotropy = 20.3636
XX= 167.4372 YX= -9.2368 ZX= 0.0907
XY= -5.9332 YY= 151.4609 ZY= -6.4926
XZ= -1.9708 YZ= -4.0053 ZZ= 151.9677
Eigenvalues: 144.6711 155.6637 170.5310
11 O Isotropic = 85.7670 Anisotropy = 151.3535
XX= -19.1517 YX= 104.3291 ZX= 84.7370
XY= 58.8516 YY= 152.0025 ZY= -22.1796
XZ= 107.6503 YZ= -41.4200 ZZ= 124.4502
Eigenvalues: -97.8427 168.4744 186.6693
12 C Isotropic = 13.1190 Anisotropy = 75.9396
XX= 57.0188 YX= -12.3747 ZX= -1.2580
XY= 2.4560 YY= -69.1768 ZY= 25.5164
XZ= -9.7229 YZ= 29.6861 ZZ= 51.5150
Eigenvalues: -75.2919 50.9035 63.7453
13 C Isotropic = 41.5881 Anisotropy = 146.6976
XX= 26.3277 YX= 62.8337 ZX= 76.4392
XY= 57.5765 YY= 34.6004 ZY= -6.1088
XZ= 81.7884 YZ= -1.5119 ZZ= 63.8363
Eigenvalues: -63.1064 48.4843 139.3865
14 O Isotropic = 237.2370 Anisotropy = 172.3556
XX= 294.7087 YX= 38.9540 ZX= 19.7303
XY= 47.7258 YY= 75.9426 ZY= 10.5687
XZ= 24.3429 YZ= 6.7417 ZZ= 341.0597
Eigenvalues: 67.5989 291.9713 352.1407
15 O Isotropic = -67.1054 Anisotropy = 587.6007
XX= -137.1386 YX= 12.8778 ZX= 289.8361
XY= 16.9779 YY= -203.1899 ZY= 107.1265
XZ= 256.5392 YZ= 100.1830 ZZ= 139.0124
Eigenvalues: -321.8043 -204.1402 324.6284
16 C Isotropic = 60.4932 Anisotropy = 172.3705
XX= 49.0907 YX= 58.2670 ZX= 89.7599
XY= 57.8417 YY= 49.9065 ZY= -0.2731
XZ= 100.9236 YZ= 3.6616 ZZ= 82.4823

Eigenvalues: -51.0208 57.0935 175.4068
17 C Isotropic = 164.2059 Anisotropy = 29.5960
XX= 159.1381 YX= -5.7223 ZX= -5.4895
XY= 1.1506 YY= 150.3349 ZY= 0.3865
XZ= -2.5225 YZ= 3.2708 ZZ= 183.1447
Eigenvalues: 149.7551 158.9261 183.9366
18 C Isotropic = 162.5318 Anisotropy = 39.2612
XX= 164.1666 YX= -10.1735 ZX= -12.7217
XY= -11.6362 YY= 170.6388 ZY= 13.4860
XZ= -13.2589 YZ= 14.1573 ZZ= 152.7901
Eigenvalues: 142.6231 156.2665 188.7060
19 H Isotropic = 29.3965 Anisotropy = 3.9386
XX= 28.8948 YX= 1.8470 ZX= -0.0734
XY= 1.0892 YY= 28.2194 ZY= -0.6099
XZ= -1.9647 YZ= -1.2006 ZZ= 31.0753
Eigenvalues: 27.0491 29.1182 32.0222
20 H Isotropic = 29.8497 Anisotropy = 10.9980
XX= 29.5161 YX= -0.4715 ZX= 5.2670
XY= -0.4415 YY= 27.2364 ZY= 0.4714
XZ= 6.3014 YZ= 1.1204 ZZ= 32.7965
Eigenvalues: 24.8448 27.5226 37.1816
21 H Isotropic = 30.0665 Anisotropy = 7.1813
XX= 32.7734 YX= 3.1369 ZX= 0.5925
XY= 3.4124 YY= 29.3685 ZY= -1.1922
XZ= 2.3938 YZ= -0.7515 ZZ= 28.0577
Eigenvalues: 26.0505 29.2950 34.8541
22 H Isotropic = 30.2750 Anisotropy = 8.5730
XX= 27.3049 YX= -0.4241 ZX= 2.1244
XY= -1.0701 YY= 32.4472 ZY= 3.8721
XZ= 2.6748 YZ= 4.2349 ZZ= 31.0730
Eigenvalues: 25.1071 29.7276 35.9903
23 H Isotropic = 28.9452 Anisotropy = 4.8226
XX= 27.2941 YX= 2.6713 ZX= 2.1032
XY= 1.3689 YY= 27.5025 ZY= 0.2637
XZ= -1.0536 YZ= -1.6934 ZZ= 32.0389
Eigenvalues: 25.2630 29.4123 32.1602
24 H Isotropic = 26.1761 Anisotropy = 3.9231
XX= 26.2456 YX= -1.1867 ZX= 0.9643
XY= -0.0764 YY= 27.6277 ZY= 2.3524
XZ= 2.3967 YZ= 1.9736 ZZ= 24.6551
Eigenvalues: 22.6359 27.1009 28.7915
25 H Isotropic = 27.5909 Anisotropy = 3.1745
XX= 28.5926 YX= 0.5565 ZX= 0.1232
XY= 0.4011 YY= 25.4543 ZY= -1.2857
XZ= 1.4612 YZ= -1.9979 ZZ= 28.7257
Eigenvalues: 24.6298 28.4356 29.7072
26 H Isotropic = 28.3972 Anisotropy = 8.2966
XX= 27.7050 YX= 0.5222 ZX= 4.8295

XY= 0.1344 YY= 26.3794 ZY= 1.8637
XZ= 2.8711 YZ= 1.3662 ZZ= 31.1072
Eigenvalues: 24.8943 26.3690 33.9283
27 H Isotropic = 30.3167 Anisotropy = 4.0925
XX= 31.1208 YX= 0.5916 ZX= -2.0051
XY= -0.0748 YY= 29.9685 ZY= -1.7115
XZ= -2.1155 YZ= -1.1851 ZZ= 29.8608
Eigenvalues: 27.8061 30.0989 33.0450
28 H Isotropic = 29.4298 Anisotropy = 8.4819
XX= 27.9213 YX= -0.3843 ZX= 1.7810
XY= -0.5127 YY= 31.9540 ZY= 3.9209
XZ= 1.6250 YZ= 5.1098 ZZ= 28.4142
Eigenvalues: 24.5172 28.6879 35.0844
29 H Isotropic = 29.7831 Anisotropy = 8.3115
XX= 29.3683 YX= 0.5867 ZX= 0.0359
XY= 1.7571 YY= 32.4444 ZY= -3.7602
XZ= -0.2943 YZ= -5.2714 ZZ= 27.5366
Eigenvalues: 24.7976 29.2275 35.3241
30 H Isotropic = 29.2900 Anisotropy = 3.0532
XX= 29.7986 YX= -0.8874 ZX= -0.0377
XY= 1.1082 YY= 29.6409 ZY= 1.7001
XZ= 1.8617 YZ= 2.1380 ZZ= 28.4305
Eigenvalues: 26.8652 29.6793 31.3255
31 H Isotropic = 26.1605 Anisotropy = 7.8224
XX= 26.4119 YX= 4.1040 ZX= -0.8838
XY= 2.7855 YY= 27.5995 ZY= -1.8365
XZ= -0.2922 YZ= -3.5016 ZZ= 24.4703
Eigenvalues: 22.3551 24.7511 31.3754
32 H Isotropic = 25.0578 Anisotropy = 5.0483
XX= 24.9472 YX= 0.9691 ZX= -0.0207
XY= 2.3664 YY= 26.9435 ZY= -2.6093
XZ= 0.3622 YZ= -1.2900 ZZ= 23.2827
Eigenvalues: 22.1601 24.5900 28.4233
33 H Isotropic = 30.3652 Anisotropy = 10.0251
XX= 29.7147 YX= 3.7461 ZX= -2.2838
XY= 3.6419 YY= 31.3666 ZY= -2.7532
XZ= -3.8180 YZ= -3.5608 ZZ= 30.0142
Eigenvalues: 26.5832 27.4637 37.0486
34 H Isotropic = 31.0845 Anisotropy = 8.0110
XX= 30.4886 YX= 1.6476 ZX= 1.2581
XY= 1.4099 YY= 26.7836 ZY= -0.6352
XZ= 1.9676 YZ= -0.6574 ZZ= 35.9811
Eigenvalues: 26.0948 30.7334 36.4251
35 H Isotropic = 30.3138 Anisotropy = 6.0766
XX= 30.0901 YX= -3.2456 ZX= -1.8365
XY= -2.8186 YY= 31.7250 ZY= -0.8444
XZ= -3.1738 YZ= 0.0068 ZZ= 29.1262
Eigenvalues: 26.0383 30.5382 34.3648

36 H Isotropic = 30.0233 Anisotropy = 7.8525
XX= 34.6269 YX= -0.5385 ZX= -0.5453
XY= -2.3876 YY= 28.8547 ZY= 1.6063
XZ= -1.9727 YZ= 1.1762 ZZ= 26.5883
Eigenvalues: 25.8938 28.9177 35.2583
37 H Isotropic = 29.7942 Anisotropy = 5.6293
XX= 29.2557 YX= -2.2970 ZX= -0.5209
XY= -1.9490 YY= 27.7030 ZY= 2.2077
XZ= 0.5600 YZ= 2.4523 ZZ= 32.4239
Eigenvalues: 25.6456 30.1899 33.5471
38 H Isotropic = 30.1722 Anisotropy = 9.0951
XX= 28.3019 YX= -1.8746 ZX= -0.7921
XY= -0.6608 YY= 35.9222 ZY= -1.0880
XZ= -0.1020 YZ= -1.1524 ZZ= 26.2926
Eigenvalues: 26.0031 28.2780 36.2357

RRRSZ

1 C Isotropic = 157.6008 Anisotropy = 17.2619
XX= 155.9683 YX= -6.7698 ZX= 10.5383
XY= -8.9784 YY= 162.8756 ZY= 1.7898
XZ= 6.6633 YZ= 0.9229 ZZ= 153.9584
Eigenvalues: 144.0770 159.6165 169.1087
2 C Isotropic = 144.5850 Anisotropy = 41.5471
XX= 169.7415 YX= 0.8193 ZX= 7.9362
XY= 3.3374 YY= 134.4833 ZY= 8.6102
XZ= 11.2548 YZ= 6.3957 ZZ= 129.5303
Eigenvalues: 123.1157 138.3563 172.2831
3 C Isotropic = 122.3091 Anisotropy = 59.2383
XX= 129.9269 YX= -6.6965 ZX= 42.6170
XY= -6.9130 YY= 132.9403 ZY= 7.9527
XZ= 43.0536 YZ= 5.9473 ZZ= 104.0600
Eigenvalues: 70.7543 134.3716 161.8012
4 C Isotropic = 125.8519 Anisotropy = 45.2034
XX= 135.2414 YX= -2.9973 ZX= 26.3860
XY= -0.9700 YY= 134.5798 ZY= 5.7466
XZ= 35.7043 YZ= 12.5363 ZZ= 107.7345
Eigenvalues: 85.9552 135.6131 155.9875
5 C Isotropic = 40.0101 Anisotropy = 174.7090
XX= 64.2799 YX= -13.8620 ZX= 76.1432
XY= -11.0635 YY= 38.0399 ZY= -86.8032
XZ= 72.9043 YZ= -84.5700 ZZ= 17.7104
Eigenvalues: -76.7240 40.2716 156.4827
6 C Isotropic = 56.6594 Anisotropy = 121.5484
XX= 65.3090 YX= 4.6594 ZX= 66.5541
XY= -0.8874 YY= 79.2416 ZY= -56.5879
XZ= 66.9739 YZ= -55.7016 ZZ= 25.4275

Eigenvalues: -42.7520 75.0384 137.6916
7 C Isotropic = 107.2389 Anisotropy = 48.5146
XX= 110.0330 YX= -3.1932 ZX= 26.5476
XY= -0.6906 YY= 97.8140 ZY= -14.0698
XZ= 22.6952 YZ= -12.1144 ZZ= 113.8698
Eigenvalues: 82.8737 99.2610 139.5819
8 C Isotropic = 138.3633 Anisotropy = 18.7414
XX= 149.0900 YX= 4.0260 ZX= 8.5761
XY= -5.5269 YY= 137.3105 ZY= 4.9797
XZ= 3.6592 YZ= 7.4717 ZZ= 128.6895
Eigenvalues: 124.0823 140.1502 150.8576
9 C Isotropic = 151.5756 Anisotropy = 35.5470
XX= 174.0027 YX= -6.4458 ZX= 1.2525
XY= -1.5869 YY= 144.5829 ZY= 10.2700
XZ= -9.5077 YZ= 6.6770 ZZ= 136.1410
Eigenvalues: 130.8485 148.6046 175.2736
10 C Isotropic = 154.1158 Anisotropy = 28.0146
XX= 164.8251 YX= -15.9855 ZX= -8.0057
XY= -13.2913 YY= 142.7187 ZY= -3.3468
XZ= -1.8993 YZ= -1.0850 ZZ= 154.8037
Eigenvalues: 134.5482 155.0070 172.7923
11 O Isotropic = 99.5020 Anisotropy = 174.1506
XX= 120.1699 YX= 83.5968 ZX= -136.2287
XY= 64.2699 YY= 158.3247 ZY= 69.6567
XZ= -89.1124 YZ= 104.7505 ZZ= 20.0114
Eigenvalues: -102.6274 185.5310 215.6024
12 C Isotropic = 14.4856 Anisotropy = 78.7046
XX= 40.1073 YX= -57.5769 ZX= 18.3436
XY= -50.1611 YY= -45.2503 ZY= 19.2610
XZ= 3.1305 YZ= 8.6009 ZZ= 48.5999
Eigenvalues: -73.7229 50.2244 66.9554
13 C Isotropic = 35.5335 Anisotropy = 146.1342
XX= 27.5826 YX= 15.5958 ZX= -67.3568
XY= 17.3273 YY= 36.1254 ZY= 77.1320
XZ= -51.0535 YZ= 87.7058 ZZ= 42.8925
Eigenvalues: -72.4195 46.0636 132.9563
14 O Isotropic = 248.9054 Anisotropy = 160.1870
XX= 344.7728 YX= 14.2756 ZX= 18.5254
XY= 41.8679 YY= 81.5654 ZY= 15.2161
XZ= 8.6778 YZ= 36.7524 ZZ= 320.3780
Eigenvalues: 76.1544 314.8651 355.6968
15 O Isotropic = -66.2812 Anisotropy = 593.4467
XX= -90.5740 YX= -154.3682 ZX= -256.5836
XY= -164.5016 YY= -113.8650 ZY= 130.7388
XZ= -289.6737 YZ= 134.7736 ZZ= 5.5953
Eigenvalues: -329.3676 -198.8260 329.3499
16 C Isotropic = 60.4435 Anisotropy = 166.5308
XX= 34.8245 YX= 13.3003 ZX= -77.6532

XY= 14.8048 YY= 58.5437 ZY= 81.2345
XZ= -70.4047 YZ= 73.0949 ZZ= 87.9621
Eigenvalues: -50.7138 60.5801 171.4640
17 C Isotropic = 165.1938 Anisotropy = 31.5758
XX= 163.8040 YX= -1.4090 ZX= 11.5531
XY= 3.7133 YY= 151.7244 ZY= -0.3878
XZ= 11.0619 YZ= 7.4752 ZZ= 180.0530
Eigenvalues: 151.2808 158.0563 186.2444
18 C Isotropic = 162.2535 Anisotropy = 39.2768
XX= 147.4580 YX= 0.3573 ZX= -7.9635
XY= -1.4413 YY= 174.2872 ZY= 17.4111
XZ= -8.7748 YZ= 17.4166 ZZ= 165.0152
Eigenvalues: 142.4509 155.8715 188.4380
19 H Isotropic = 29.3269 Anisotropy = 4.3921
XX= 28.3483 YX= 0.8228 ZX= 2.1490
XY= 0.1612 YY= 27.9846 ZY= -0.8767
XZ= -0.0056 YZ= -1.6894 ZZ= 31.6477
Eigenvalues: 27.0385 28.6872 32.2549
20 H Isotropic = 29.8049 Anisotropy = 10.9660
XX= 36.0880 YX= 0.3021 ZX= 2.8983
XY= -0.0913 YY= 27.3666 ZY= 0.4377
XZ= 3.8404 YZ= 0.9248 ZZ= 25.9603
Eigenvalues: 24.7913 27.5079 37.1156
21 H Isotropic = 29.9751 Anisotropy = 6.9090
XX= 32.6678 YX= 1.7279 ZX= -2.6498
XY= 1.8412 YY= 28.6988 ZY= -2.8663
XZ= -0.9044 YZ= -2.4068 ZZ= 28.5587
Eigenvalues: 25.9911 29.3531 34.5811
22 H Isotropic = 30.2114 Anisotropy = 8.3500
XX= 30.9508 YX= 2.3308 ZX= 2.4335
XY= 1.5644 YY= 32.8096 ZY= 3.1276
XZ= 2.7871 YZ= 2.8542 ZZ= 26.8738
Eigenvalues: 25.0764 29.7797 35.7781
23 H Isotropic = 28.8288 Anisotropy = 7.5134
XX= 28.9051 YX= 0.8924 ZX= 5.0869
XY= 0.7544 YY= 26.5336 ZY= 0.0351
XZ= 2.2703 YZ= -2.4186 ZZ= 31.0478
Eigenvalues: 24.9415 27.7073 33.8378
24 H Isotropic = 26.1492 Anisotropy = 3.9754
XX= 27.3734 YX= 0.1877 ZX= -0.6627
XY= 1.2509 YY= 27.9783 ZY= 1.5705
XZ= 0.4497 YZ= 1.7684 ZZ= 23.0959
Eigenvalues: 22.5588 27.0893 28.7995
25 H Isotropic = 26.9528 Anisotropy = 6.2680
XX= 26.2166 YX= -1.2167 ZX= -2.8451
XY= -0.4603 YY= 25.3442 ZY= 1.7694
XZ= -0.7924 YZ= 2.7293 ZZ= 29.2976
Eigenvalues: 24.3262 25.4007 31.1315

26 H Isotropic = 28.7577 Anisotropy = 6.6421
XX= 28.1414 YX= 0.1267 ZX= -2.6297
XY= 1.3853 YY= 26.7687 ZY= -1.3241
XZ= -1.8131 YZ= -2.6247 ZZ= 31.3629
Eigenvalues: 26.0334 27.0539 33.1857
27 H Isotropic = 30.2385 Anisotropy = 7.0833
XX= 32.4507 YX= 2.0119 ZX= 0.6427
XY= 0.9401 YY= 33.0387 ZY= 2.2749
XZ= 0.3750 YZ= 3.4993 ZZ= 25.2262
Eigenvalues: 24.2750 31.4798 34.9607
28 H Isotropic = 30.1928 Anisotropy = 2.2976
XX= 30.1892 YX= 0.0278 ZX= -0.9741
XY= -1.5205 YY= 30.4184 ZY= -1.0799
XZ= -2.1863 YZ= -1.1496 ZZ= 29.9708
Eigenvalues: 27.8185 31.0354 31.7245
29 H Isotropic = 29.7383 Anisotropy = 8.6127
XX= 27.8869 YX= -1.6632 ZX= 1.3021
XY= -0.7060 YY= 32.2054 ZY= -4.0294
XZ= -0.6605 YZ= -4.7254 ZZ= 29.1225
Eigenvalues: 25.9249 27.8098 35.4801
30 H Isotropic = 29.1381 Anisotropy = 2.9940
XX= 29.6927 YX= 0.2183 ZX= 0.3554
XY= 1.5022 YY= 30.0710 ZY= 0.0463
XZ= 1.2219 YZ= 1.6030 ZZ= 27.6505
Eigenvalues: 27.2744 29.0057 31.1341
31 H Isotropic = 26.0634 Anisotropy = 7.3346
XX= 28.3574 YX= 4.5285 ZX= -2.0461
XY= 2.6167 YY= 25.7667 ZY= 0.2149
XZ= -0.4732 YZ= 0.6513 ZZ= 24.0662
Eigenvalues: 22.4894 24.7478 30.9532
32 H Isotropic = 25.2415 Anisotropy = 5.6160
XX= 26.1644 YX= 2.2573 ZX= -0.7749
XY= 3.6787 YY= 25.7682 ZY= 0.6798
XZ= -0.9164 YZ= -0.2690 ZZ= 23.7920
Eigenvalues: 22.5520 24.1871 28.9855
33 H Isotropic = 30.1099 Anisotropy = 8.8393
XX= 35.3727 YX= 1.4958 ZX= 1.5239
XY= 1.1182 YY= 23.9760 ZY= -0.6563
XZ= 1.8065 YZ= -1.4421 ZZ= 30.9809
Eigenvalues: 23.6170 30.7099 36.0027
34 H Isotropic = 30.4353 Anisotropy = 5.6941
XX= 27.9554 YX= -2.4227 ZX= -0.2666
XY= -2.8724 YY= 32.0468 ZY= 0.8096
XZ= -1.8105 YZ= 1.7448 ZZ= 31.3036
Eigenvalues: 26.6236 30.4509 34.2313
35 H Isotropic = 30.4538 Anisotropy = 9.9382
XX= 27.4940 YX= 1.2819 ZX= -0.2888
XY= 1.4161 YY= 30.1970 ZY= -4.0601

XZ= -2.1267 YZ= -4.9372 ZZ= 33.6703
Eigenvalues: 26.7177 27.5644 37.0793
36 H Isotropic = 30.0206 Anisotropy = 7.8164
XX= 30.7039 YX= -0.2085 ZX= -3.2295
XY= -1.6487 YY= 29.3751 ZY= 3.0026
XZ= -4.7896 YZ= 1.5563 ZZ= 29.9828
Eigenvalues: 25.9279 28.9023 35.2315
37 H Isotropic = 30.1755 Anisotropy = 9.1854
XX= 27.1379 YX= -1.8767 ZX= -1.0811
XY= -0.8291 YY= 36.0125 ZY= -1.3730
XZ= -0.7503 YZ= -0.6491 ZZ= 27.3762
Eigenvalues: 26.0489 28.1786 36.2991
38 H Isotropic = 29.8405 Anisotropy = 5.2661
XX= 30.7102 YX= -0.5097 ZX= 1.3169
XY= -0.4519 YY= 28.4058 ZY= 3.0718
XZ= 2.1130 YZ= 3.5192 ZZ= 30.4056
Eigenvalues: 25.5641 30.6062 33.3513

RSRRZ

1 C Isotropic = 161.6181 Anisotropy = 16.4765
XX= 162.6050 YX= -2.8764 ZX= 8.7518
XY= -4.5895 YY= 169.2486 ZY= 7.3357
XZ= 10.8698 YZ= 8.8338 ZZ= 153.0007
Eigenvalues: 143.8057 168.4461 172.6024
2 C Isotropic = 152.9464 Anisotropy = 23.6230
XX= 147.5146 YX= -15.3181 ZX= 11.0972
XY= -8.8155 YY= 154.6579 ZY= -3.0027
XZ= 6.0915 YZ= -2.8478 ZZ= 156.6666
Eigenvalues: 137.0006 153.1434 168.6951
3 C Isotropic = 125.4549 Anisotropy = 55.1577
XX= 79.0424 YX= -8.6858 ZX= -11.5466
XY= -13.3436 YY= 142.0931 ZY= -11.7585
XZ= -11.7452 YZ= -11.3490 ZZ= 155.2291
Eigenvalues: 74.8970 139.2410 162.2267
4 C Isotropic = 119.4702 Anisotropy = 52.0434
XX= 89.0271 YX= 0.9388 ZX= -12.9482
XY= 4.7879 YY= 126.6789 ZY= -9.4666
XZ= -16.8813 YZ= -18.8973 ZZ= 142.7044
Eigenvalues: 85.1451 119.0996 154.1657
5 C Isotropic = 39.3311 Anisotropy = 172.6583
XX= 85.1314 YX= -40.3387 ZX= 42.0750
XY= -33.7436 YY= 55.9775 ZY= -88.8893
XZ= 45.7828 YZ= -81.1915 ZZ= -23.1155
Eigenvalues: -79.3271 42.8838 154.4367
6 C Isotropic = 55.0980 Anisotropy = 123.7525
XX= 94.2715 YX= -13.6495 ZX= 42.4092

XY= -13.5517 YY= 84.3752 ZY= -60.0752
XZ= 40.7069 YZ= -61.3279 ZZ= -13.3526
Eigenvalues: -49.6385 77.3329 137.5997
7 C Isotropic = 103.2282 Anisotropy = 43.4467
XX= 123.4952 YX= -12.0261 ZX= -0.8428
XY= -17.4442 YY= 106.6292 ZY= -0.6562
XZ= -7.2079 YZ= -1.9498 ZZ= 79.5603
Eigenvalues: 78.8939 98.5981 132.1927
8 C Isotropic = 145.9414 Anisotropy = 25.3060
XX= 156.7028 YX= 8.8023 ZX= 6.0551
XY= 4.9371 YY= 148.5364 ZY= 0.8714
XZ= 10.1151 YZ= 3.5663 ZZ= 132.5852
Eigenvalues: 130.1247 144.8875 162.8121
9 C Isotropic = 150.5332 Anisotropy = 26.8487
XX= 154.1582 YX= -3.4435 ZX= 7.6103
XY= 0.3603 YY= 155.6976 ZY= -11.4656
XZ= 15.9658 YZ= -15.1824 ZZ= 141.7439
Eigenvalues: 129.8742 153.2932 168.4324
10 C Isotropic = 155.7533 Anisotropy = 14.6994
XX= 158.3732 YX= -13.2863 ZX= -5.8543
XY= -6.8035 YY= 147.5045 ZY= -7.1274
XZ= -3.7106 YZ= -2.2870 ZZ= 161.3822
Eigenvalues: 139.5752 162.1318 165.5529
11 O Isotropic = 90.7856 Anisotropy = 164.6669
XX= -4.8580 YX= 158.3255 ZX= 32.3680
XY= 112.5339 YY= 106.9123 ZY= -15.5503
XZ= 24.0737 YZ= -0.1958 ZZ= 170.3027
Eigenvalues: -98.3664 170.1597 200.5636
12 C Isotropic = 13.5088 Anisotropy = 77.9087
XX= 48.5837 YX= -47.4565 ZX= -19.8274
XY= -33.9774 YY= -34.2047 ZY= -42.5372
XZ= -11.9309 YZ= -45.5893 ZZ= 26.1474
Eigenvalues: -72.9721 48.0505 65.4479
13 C Isotropic = 37.9684 Anisotropy = 142.3426
XX= -3.9124 YX= 67.2731 ZX= -0.0814
XY= 61.7982 YY= 10.5609 ZY= -42.6818
XZ= -6.5480 YZ= -51.0338 ZZ= 107.2566
Eigenvalues: -66.6692 47.7108 132.8635
14 O Isotropic = 256.6034 Anisotropy = 152.0455
XX= 314.7321 YX= 34.5087 ZX= -6.3327
XY= 27.1205 YY= 132.3976 ZY= -84.3335
XZ= -11.2716 YZ= -68.2827 ZZ= 322.6805
Eigenvalues: 102.3353 309.5078 357.9671
15 O Isotropic = -59.6985 Anisotropy = 579.9108
XX= -291.9073 YX= 19.9436 ZX= -104.6266
XY= 23.5429 YY= -116.2711 ZY= -186.8920
XZ= -102.4436 YZ= -183.2757 ZZ= 229.0829
Eigenvalues: -313.0645 -192.9397 326.9087

16 C Isotropic = 59.3284 Anisotropy = 172.6110
XX= -6.2011 YX= 62.4971 ZX= -12.0264
XY= 66.2161 YY= 33.1396 ZY= -46.5377
XZ= -13.1709 YZ= -47.6276 ZZ= 151.0466
Eigenvalues: -55.4961 59.0789 174.4024
17 C Isotropic = 164.4168 Anisotropy = 38.9719
XX= 164.3622 YX= 0.6914 ZX= -15.7221
XY= 4.8960 YY= 151.4089 ZY= -13.0168
XZ= -12.9510 YZ= -11.7909 ZZ= 177.4795
Eigenvalues: 145.8719 156.9805 190.3981
18 C Isotropic = 162.7564 Anisotropy = 37.5489
XX= 147.0372 YX= 4.8569 ZX= 1.0224
XY= 4.7718 YY= 173.8684 ZY= 16.1924
XZ= -0.3620 YZ= 16.7558 ZZ= 167.3635
Eigenvalues: 145.7007 154.7793 187.7890
19 H Isotropic = 29.6947 Anisotropy = 8.5016
XX= 34.8861 YX= 1.1242 ZX= -2.7068
XY= 0.5799 YY= 28.2509 ZY= 0.4890
XZ= -1.1927 YZ= 0.8249 ZZ= 25.9471
Eigenvalues: 25.3095 28.4122 35.3624
20 H Isotropic = 29.3732 Anisotropy = 9.0636
XX= 29.4547 YX= -1.2530 ZX= 5.5027
XY= -1.9780 YY= 28.6016 ZY= -1.8044
XZ= 3.9314 YZ= -2.0659 ZZ= 30.0633
Eigenvalues: 25.0249 27.6791 35.4156
21 H Isotropic = 29.9315 Anisotropy = 4.3391
XX= 29.9817 YX= 0.8656 ZX= -0.9692
XY= -0.1900 YY= 27.9950 ZY= -1.0679
XZ= -0.9748 YZ= -2.2946 ZZ= 31.8176
Eigenvalues: 27.3605 29.6097 32.8242
22 H Isotropic = 29.9089 Anisotropy = 8.5663
XX= 29.4123 YX= 1.6680 ZX= 2.5581
XY= 1.8982 YY= 31.7243 ZY= 3.1384
XZ= 4.0344 YZ= 3.4203 ZZ= 28.5901
Eigenvalues: 25.3273 28.7796 35.6198
23 H Isotropic = 29.3782 Anisotropy = 6.6132
XX= 28.0274 YX= 3.2544 ZX= 0.1089
XY= 2.2970 YY= 27.2008 ZY= -2.6744
XZ= 3.5300 YZ= -1.6132 ZZ= 32.9064
Eigenvalues: 23.9273 30.4203 33.7870
24 H Isotropic = 25.9368 Anisotropy = 5.3219
XX= 26.9515 YX= 1.5185 ZX= -1.3273
XY= 2.2116 YY= 27.9759 ZY= 1.1104
XZ= -0.0930 YZ= 1.8002 ZZ= 22.8831
Eigenvalues: 22.1840 26.1417 29.4847
25 H Isotropic = 27.7900 Anisotropy = 3.8197
XX= 29.8268 YX= -0.9197 ZX= 0.9071
XY= -1.2189 YY= 26.6976 ZY= -0.8674

XZ= 0.3687 YZ= -0.3321 ZZ= 26.8455
Eigenvalues: 26.1122 26.9213 30.3364
 26 H Isotropic = 29.0623 Anisotropy = 2.9140
XX= 29.9646 YX= -0.7131 ZX= -1.2144
XY= 0.0722 YY= 28.6396 ZY= 0.4747
XZ= -1.6163 YZ= 0.7756 ZZ= 28.5828
Eigenvalues: 27.5641 28.6179 31.0050
 27 H Isotropic = 30.1310 Anisotropy = 7.0679
XX= 30.8917 YX= 0.1024 ZX= -3.7401
XY= -0.2271 YY= 27.5484 ZY= -2.1477
XZ= -2.2515 YZ= -2.1947 ZZ= 31.9531
Eigenvalues: 26.2501 29.3000 34.8430
 28 H Isotropic = 29.7951 Anisotropy = 7.1238
XX= 30.3539 YX= 2.4366 ZX= 1.0908
XY= 1.6869 YY= 33.3592 ZY= 1.1871
XZ= 0.9773 YZ= 0.2205 ZZ= 25.6721
Eigenvalues: 25.4440 29.3969 34.5443
 29 H Isotropic = 29.7836 Anisotropy = 10.1485
XX= 28.0395 YX= -2.3881 ZX= 1.9742
XY= -1.3892 YY= 31.1903 ZY= -4.9394
XZ= 1.2590 YZ= -5.3406 ZZ= 30.1212
Eigenvalues: 25.4860 27.3157 36.5493
 30 H Isotropic = 29.1487 Anisotropy = 4.5312
XX= 29.0014 YX= 2.0546 ZX= 0.2986
XY= 2.5853 YY= 29.4752 ZY= 0.4731
XZ= 1.5854 YZ= 1.5569 ZZ= 28.9694
Eigenvalues: 26.9061 28.3705 32.1695
 31 H Isotropic = 26.0802 Anisotropy = 7.8065
XX= 27.7749 YX= 4.4101 ZX= 3.0977
XY= 2.1624 YY= 24.8000 ZY= 0.7611
XZ= 2.1314 YZ= 1.4163 ZZ= 25.6657
Eigenvalues: 22.5571 24.3989 31.2846
 32 H Isotropic = 25.0915 Anisotropy = 5.2761
XX= 25.2035 YX= 1.6350 ZX= 1.0510
XY= 3.5183 YY= 25.3949 ZY= 1.2957
XZ= 1.4959 YZ= 0.9584 ZZ= 24.6761
Eigenvalues: 22.7079 23.9578 28.6089
 33 H Isotropic = 31.1582 Anisotropy = 10.3573
XX= 29.0947 YX= -0.3900 ZX= 0.1692
XY= -0.1424 YY= 29.2690 ZY= -5.0070
XZ= 0.3031 YZ= -5.1543 ZZ= 35.1109
Eigenvalues: 26.3249 29.0866 38.0631
 34 H Isotropic = 30.2200 Anisotropy = 7.2239
XX= 28.4392 YX= -2.7389 ZX= -3.3866
XY= -1.2171 YY= 30.8581 ZY= 0.4646
XZ= -4.4925 YZ= 1.5244 ZZ= 31.3628
Eigenvalues: 25.4735 30.1506 35.0360
 35 H Isotropic = 30.3845 Anisotropy = 9.8874

XX= 32.8730 YX= 4.3590 ZX= -0.5044
XY= 4.9689 YY= 30.4098 ZY= -1.2842
XZ= -2.4411 YZ= -1.9547 ZZ= 27.8705
Eigenvalues: 26.6263 27.5510 36.9761
36 H Isotropic = 29.9989 Anisotropy = 7.3921
XX= 29.2676 YX= 0.1968 ZX= -2.4573
XY= -0.8020 YY= 29.3727 ZY= 3.6024
XZ= -4.0911 YZ= 2.1414 ZZ= 31.3564
Eigenvalues: 26.0416 29.0281 34.9270
37 H Isotropic = 30.1880 Anisotropy = 9.4462
XX= 26.8145 YX= -1.0800 ZX= -0.8358
XY= -0.0423 YY= 36.4362 ZY= -0.8489
XZ= -0.2056 YZ= 0.0060 ZZ= 27.3133
Eigenvalues: 26.4376 27.6409 36.4855
38 H Isotropic = 29.8142 Anisotropy = 5.4469
XX= 31.9901 YX= -0.4601 ZX= 1.7049
XY= -0.3238 YY= 28.2340 ZY= 2.9800
XZ= 2.3960 YZ= 3.3523 ZZ= 29.2185
Eigenvalues: 25.1200 30.8771 33.4454

DFT Structure Coordinates of four Sucrose conformers in M1 Cluster

Table S14. Coordinates of selected sucrose low energy conformers of M1 cluster.

Sucrose DFT coordinates												
Atom	Sucrose_4			Sucrose_17			Sucrose_153			Sucrose_122		
C1	-1.679	0.111	-1.303	-1.661	0.078	-1.316	-1.673	-1.281	-0.83	-1.679	0.265	-1.242
C2	-2.817	-0.854	-0.976	-2.786	-0.909	-1.011	-2.969	-0.49	-1.013	-2.747	-0.781	-0.932
C3	-2.39	-1.742	0.182	-2.346	-1.818	0.125	-2.784	0.917	-0.474	-2.237	-1.73	0.136
C4	-2.006	-0.893	1.386	-1.975	-0.993	1.351	-1.619	1.59	-1.187	-1.875	-0.923	1.377
C5	-0.956	0.143	0.982	-0.942	0.07	0.971	-0.363	0.731	-1.044	-0.864	0.165	1.008
O6	-1.388	0.894	-0.129	-1.382	0.838	-0.124	-0.588	-0.589	-1.475	-1.352	0.975	-0.035
O7	0.231	-0.545	0.66	0.253	-0.6	0.641	0.009	0.751	0.321	0.333	-0.477	0.613
C8	1.453	-0.087	1.23	1.476	-0.107	1.174	1.376	0.983	0.628	1.55	-0.05	1.216
O9	-1.561	-1.69	2.46	-1.507	-1.81	2.4	-1.408	2.901	-0.713	-1.411	-1.752	2.416
O10	-3.09	-1.629	-2.128	-3.048	-1.662	-2.18	-3.997	-1.166	-0.315	-3.056	-1.454	-2.139
C11	-2.016	1.071	-2.431	-2.01	1.058	-2.423	-1.766	-2.663	-1.455	-2.134	1.27	-2.288
O12	-3.474	-2.604	0.48	-3.418	-2.702	0.402	-3.997	1.617	-0.689	-3.268	-2.662	0.409
O13	-0.873	1.595	-3.077	-0.873	1.628	-3.04	-0.774	-3.558	-0.999	-3.397	1.851	-2.009
C14	2.54	-0.568	0.254	2.547	-0.521	0.145	1.625	0.426	2.064	2.659	-0.593	0.302
C15	2.542	0.574	-0.764	2.505	0.672	-0.814	2.872	-0.447	1.878	2.737	0.503	-0.758
C16	2.397	1.778	0.158	2.35	1.831	0.157	2.787	-0.862	0.41	2.541	1.756	0.09
O17	1.542	1.312	1.229	1.507	1.299	1.202	2.229	0.292	-0.244	1.686	1.341	1.184
C18	1.573	-0.596	2.659	1.64	-0.59	2.605	1.692	2.464	0.496	1.631	-0.543	2.654
O19	3.726	0.692	-1.514	3.668	0.842	-1.587	3.992	0.389	2.115	3.972	0.58	-1.433
O20	1.305	-1.989	2.727	1.389	-1.988	2.631	0.703	3.174	1.23	1.401	-1.945	2.713
O21	2.32	-1.857	-0.259	2.339	-1.762	-0.47	0.564	-0.358	2.555	2.427	-1.899	-0.165
C22	1.786	3.03	-0.432	1.708	3.097	-0.371	1.908	-2.077	0.156	1.896	2.932	-0.613
O23	0.487	2.811	-0.953	0.405	2.874	-0.882	1.73	-2.276	-1.242	0.676	2.591	-1.236

H24	-0.788	-0.467	-1.588		-0.762	-0.48	-1.613		-1.46	-1.382	0.244		-0.776	-0.235	-1.622
H25	-3.707	-0.276	-0.678		-3.684	-0.351	-0.701		-3.206	-0.431	-2.088		-3.639	-0.273	-0.536
H26	-1.518	-2.335	-0.14		-1.466	-2.39	-0.209		-2.571	0.856	0.605		-1.344	-2.255	-0.24
H27	-2.896	-0.355	1.734		-2.873	-0.481	1.714		-1.858	1.668	-2.253		-2.782	-0.43	1.747
H28	-0.787	0.86	1.79		-0.786	0.771	1.794		0.445	1.118	-1.67		-0.686	0.838	1.851
H29	-0.632	-1.953	2.313		-0.565	-2.019	2.253		-0.88	2.873	0.107		-0.47	-1.972	2.278
H30	-3.67	-2.354	-1.855		-3.615	-2.404	-1.923		-4.763	-0.574	-0.289		-3.625	-2.204	-1.915
H31	-2.579	0.523	-3.191		-2.55	0.516	-3.203		-2.731	-3.096	-1.18		-1.409	2.087	-2.331
H32	-2.661	1.869	-2.035		-2.679	1.83	-2.014		-1.739	-2.551	-2.549		-2.138	0.768	-3.262
H33	-3.22	-3.152	1.237		-3.15	-3.277	1.133		-3.871	2.528	-0.388		-2.981	-3.211	1.153
H34	-0.334	2.086	-2.432		-0.365	2.132	-2.379		0.107	-3.219	-1.238		-4.085	1.215	-2.246
H35	3.51	-0.585	0.764		3.529	-0.552	0.631		1.843	1.249	2.753		3.606	-0.615	0.855
H36	1.661	0.483	-1.419		1.611	0.588	-1.453		2.852	-1.304	2.561		1.904	0.39	-1.466
H37	3.383	2.029	0.573		3.332	2.084	0.578		3.775	-1.022	-0.034		3.509	2.067	0.503
H38	2.571	-0.356	3.041		2.656	-0.355	2.942		2.696	2.642	0.896		2.614	-0.28	3.062
H39	0.829	-0.099	3.29		0.924	-0.05	3.241		1.678	2.748	-0.565		0.862	-0.068	3.27
H40	3.749	-0.021	-2.168		3.708	0.127	-2.238		4.799	-0.108	1.923		4.018	-0.144	-2.073
H41	1.9	-2.455	2.121		1.611	-2.322	3.511		0.975	4.098	1.307		1.996	-2.389	2.09
H42	1.401	-1.895	-0.571		1.388	-1.849	-0.638		-0.233	-0.137	2.05		1.525	-1.927	-0.523
H43	1.761	3.81	0.339		1.678	3.842	0.434		2.394	-2.971	0.554		1.758	3.744	0.114
H44	2.417	3.382	-1.254		2.32	3.496	-1.185		0.936	-1.958	0.653		2.574	3.288	-1.394
H45	-0.044	2.304	-0.315		-0.099	2.317	-0.264		1.26	-1.492	-1.571		0.078	2.186	-0.584

Chemical Shielding Tensors of Sucrose from DFT
Sucrose_4

1 C Isotropic = 105.5763 Anisotropy = 25.2208
XX= 91.3584 YX= 13.0747 ZX= 6.9990
XY= 8.6675 YY= 108.6181 ZY= 11.5072
XZ= 2.7461 YZ= -0.9854 ZZ= 116.7523
Eigenvalues: 85.9568 108.3819 122.3902
2 C Isotropic = 115.1281 Anisotropy = 39.1337
XX= 102.2776 YX= 6.3247 ZX= 8.4642
XY= 6.3220 YY= 115.1816 ZY= 22.2499
XZ= 3.9310 YZ= 10.8230 ZZ= 127.9251
Eigenvalues: 99.6717 104.4953 141.2172
3 C Isotropic = 107.3723 Anisotropy = 22.1977
XX= 112.6306 YX= 4.4152 ZX= -2.9334
XY= 11.7316 YY= 98.8413 ZY= -4.3947
XZ= -7.5096 YZ= -10.6842 ZZ= 110.6450
Eigenvalues: 93.6004 106.3457 122.1708
4 C Isotropic = 112.1900 Anisotropy = 30.3237
XX= 107.2804 YX= 0.4671 ZX= 10.9526
XY= -6.3561 YY= 112.3626 ZY= -17.9765
XZ= 13.4931 YZ= -6.5650 ZZ= 116.9271
Eigenvalues: 97.0407 107.1236 132.4058
5 C Isotropic = 92.7273 Anisotropy = 37.9343
XX= 94.2958 YX= -9.0074 ZX= -9.6047
XY= -11.2972 YY= 87.0998 ZY= -20.8359
XZ= 3.2492 YZ= -28.9087 ZZ= 96.7863
Eigenvalues: 63.4263 96.7388 118.0169
6 O Isotropic = 217.9973 Anisotropy = 81.0971
XX= 215.8905 YX= -45.1535 ZX= -10.4241
XY= -35.2755 YY= 231.1200 ZY= -19.7241
XZ= 1.6278 YZ= -42.6677 ZZ= 206.9814
Eigenvalues: 167.1639 214.7659 272.0620
7 O Isotropic = 217.1152 Anisotropy = 46.0579
XX= 218.1963 YX= 10.4844 ZX= 5.7179
XY= -43.9482 YY= 226.0824 ZY= -14.8829
XZ= 7.6903 YZ= -21.4589 ZZ= 207.0668
Eigenvalues: 195.4977 208.0273 247.8204
8 C Isotropic = 83.7752 Anisotropy = 21.2206
XX= 86.5144 YX= 3.9176 ZX= 8.3090
XY= 8.4406 YY= 94.4972 ZY= -2.6562
XZ= 10.6908 YZ= -5.1546 ZZ= 70.3139
Eigenvalues: 64.6429 88.7603 97.9222
9 O Isotropic = 295.7503 Anisotropy = 68.2518
XX= 332.0888 YX= -29.8363 ZX= 13.7585
XY= -23.1823 YY= 264.2373 ZY= -2.5069
XZ= -15.5299 YZ= -10.6158 ZZ= 290.9248
Eigenvalues: 253.9674 292.0320 341.2515
10 O Isotropic = 292.7381 Anisotropy = 37.0620
XX= 279.8483 YX= 0.6076 ZX= -20.9364
XY= 15.3173 YY= 315.1244 ZY= 19.0019
XZ= -7.1093 YZ= -4.4808 ZZ= 283.2417
Eigenvalues: 265.0991 295.6692 317.4461
11 C Isotropic = 122.4052 Anisotropy = 51.3001

XX= 136.6025 YX= 11.1500 ZX= -20.1738
XY= 12.2060 YY= 114.2874 ZY= -20.6570
XZ= -14.7178 YZ= -18.6307 ZZ= 116.3258
Eigenvalues: 95.2261 115.3843 156.6053
12 O Isotropic = 296.2666 Anisotropy = 47.2563
XX= 317.9932 YX= 10.1983 ZX= -9.7549
XY= -26.3300 YY= 275.5966 ZY= -17.4645
XZ= -23.7905 YZ= -36.4733 ZZ= 295.2100
Eigenvalues: 252.5946 308.4344 327.7708
13 O Isotropic = 294.5781 Anisotropy = 27.0333
XX= 302.1289 YX= -2.3623 ZX= 2.0198
XY= -10.6534 YY= 288.0744 ZY= -10.0351
XZ= 18.6811 YZ= -4.0081 ZZ= 293.5309
Eigenvalues: 283.2446 287.8894 312.6003
14 C Isotropic = 99.7805 Anisotropy = 27.2228
XX= 83.8772 YX= 2.2398 ZX= -11.7495
XY= 7.3962 YY= 116.4175 ZY= 0.0177
XZ= -4.8109 YZ= -5.1575 ZZ= 99.0468
Eigenvalues: 79.9139 101.4985 117.9290
15 C Isotropic = 110.7812 Anisotropy = 40.5677
XX= 111.8815 YX= 3.0340 ZX= -16.2346
XY= -2.8076 YY= 110.3843 ZY= -8.2197
XZ= -32.7528 YZ= -14.0975 ZZ= 110.0778
Eigenvalues: 83.9613 110.5561 137.8263
16 C Isotropic = 102.4494 Anisotropy = 52.5808
XX= 99.2599 YX= 8.6218 ZX= -34.2503
XY= -3.0842 YY= 94.1525 ZY= -10.1413
XZ= -22.6394 YZ= -6.1373 ZZ= 113.9359
Eigenvalues: 76.7419 93.1031 137.5032
17 O Isotropic = 237.0594 Anisotropy = 101.3371
XX= 184.9266 YX= -10.6270 ZX= -9.3317
XY= -6.6991 YY= 303.4027 ZY= -6.0377
XZ= -21.3859 YZ= -9.8819 ZZ= 222.8487
Eigenvalues: 178.5451 228.0155 304.6175
18 C Isotropic = 117.9191 Anisotropy = 48.1290
XX= 98.7035 YX= 13.2283 ZX= 4.1082
XY= 7.5439 YY= 144.2411 ZY= -11.8477
XZ= 3.7293 YZ= -13.6053 ZZ= 110.8127
Eigenvalues: 93.5483 110.2039 150.0051
19 O Isotropic = 299.8660 Anisotropy = 37.8733
XX= 316.0063 YX= 5.5166 ZX= -9.6985
XY= -18.3248 YY= 292.6645 ZY= 34.7112
XZ= 11.7468 YZ= 28.4460 ZZ= 290.9274
Eigenvalues: 259.7230 314.7602 325.1149
20 O Isotropic = 298.5306 Anisotropy = 51.8292
XX= 299.0850 YX= -35.5367 ZX= -15.4013
XY= -8.2775 YY= 285.7717 ZY= 4.7777
XZ= -12.7873 YZ= 23.8737 ZZ= 310.7351
Eigenvalues: 269.2377 293.2707 333.0834
21 O Isotropic = 294.4179 Anisotropy = 56.7162
XX= 324.9538 YX= 12.0027 ZX= 24.3442
XY= 0.4274 YY= 293.2930 ZY= 2.5194
XZ= 19.0633 YZ= -21.3695 ZZ= 265.0069
Eigenvalues: 254.8818 296.1431 332.2287
22 C Isotropic = 125.6382 Anisotropy = 55.7914

XX= 153.3407 YX= 5.2361 ZX= 24.3064
XY= 5.9216 YY= 114.1515 ZY= 2.9688
XZ= 18.7123 YZ= 0.8630 ZZ= 109.4226
Eigenvalues: 100.6345 113.4477 162.8325
23 O Isotropic = 305.8347 Anisotropy = 51.2731
XX= 290.1479 YX= 9.6576 ZX= -8.2816
XY= 42.1845 YY= 318.7965 ZY= -4.8881
XZ= -11.2005 YZ= -15.2480 ZZ= 308.5597
Eigenvalues: 274.5100 302.9773 340.0168
24 H Isotropic = 27.7822 Anisotropy = 3.8280
XX= 28.0113 YX= 1.7091 ZX= 1.8864
XY= -0.1468 YY= 26.2073 ZY= 0.0408
XZ= 1.0248 YZ= 1.1123 ZZ= 29.1279
Eigenvalues: 25.9156 27.0967 30.3342
25 H Isotropic = 28.4786 Anisotropy = 2.6517
XX= 29.5672 YX= -0.4234 ZX= 0.4706
XY= -1.9213 YY= 27.7986 ZY= 0.8296
XZ= 0.1049 YZ= 2.0310 ZZ= 28.0700
Eigenvalues: 26.1573 29.0322 30.2464
26 H Isotropic = 28.2134 Anisotropy = 8.3155
XX= 32.1627 YX= 2.5361 ZX= -0.8936
XY= 3.6500 YY= 27.5778 ZY= -0.2286
XZ= -0.6543 YZ= 0.7685 ZZ= 24.8996
Eigenvalues: 24.6166 26.2664 33.7570
27 H Isotropic = 28.3819 Anisotropy = 4.0356
XX= 28.9805 YX= -2.1364 ZX= -1.2931
XY= -2.9064 YY= 27.1783 ZY= 0.4226
XZ= -1.0293 YZ= -1.0024 ZZ= 28.9870
Eigenvalues: 25.1799 28.8935 31.0723
28 H Isotropic = 26.3904 Anisotropy = 2.7257
XX= 27.1165 YX= -1.0628 ZX= -1.0163
XY= -0.1304 YY= 25.2410 ZY= 1.0001
XZ= -0.1915 YZ= 1.6846 ZZ= 26.8137
Eigenvalues: 24.4524 26.5113 28.2075
29 H Isotropic = 28.2473 Anisotropy = 24.0926
XX= 43.5338 YX= -3.9258 ZX= 0.2507
XY= -4.4605 YY= 20.9702 ZY= -4.3445
XZ= -0.3165 YZ= -3.9698 ZZ= 20.2378
Eigenvalues: 16.1209 24.3119 44.3090
30 H Isotropic = 29.8830 Anisotropy = 18.1348
XX= 28.0956 YX= 11.0454 ZX= 0.9485
XY= 11.3103 YY= 32.9414 ZY= -1.6248
XZ= 0.0121 YZ= -0.3703 ZZ= 28.6119
Eigenvalues: 18.9772 28.6989 41.9729
31 H Isotropic = 27.6836 Anisotropy = 5.8568
XX= 27.9320 YX= 4.3885 ZX= 3.1737
XY= 3.8855 YY= 26.3665 ZY= -1.1061
XZ= 1.6901 YZ= -2.7748 ZZ= 28.7523
Eigenvalues: 21.6289 29.8338 31.5881
32 H Isotropic = 28.1736 Anisotropy = 5.6955
XX= 31.1244 YX= -2.8209 ZX= -1.2553
XY= -0.9872 YY= 27.6745 ZY= -2.7030
XZ= -0.9085 YZ= -1.6866 ZZ= 25.7220
Eigenvalues: 23.7684 28.7818 31.9706
33 H Isotropic = 29.7477 Anisotropy = 17.4707

XX= 25.4482 YX= 2.2422 ZX= 2.8119
XY= 3.3047 YY= 31.6660 ZY= -9.6284
XZ= 4.0131 YZ= -9.3264 ZZ= 32.1291
Eigenvalues: 19.3052 28.5432 41.3949
34 H Isotropic = 27.5474 Anisotropy = 26.3956
XX= 27.6307 YX= 10.1701 ZX= 10.6446
XY= 10.0635 YY= 23.5522 ZY= 5.5835
XZ= 8.7667 YZ= 6.0786 ZZ= 31.4594
Eigenvalues: 15.0149 22.4828 45.1445
35 H Isotropic = 27.8625 Anisotropy = 2.9774
XX= 29.1401 YX= -0.9477 ZX= 0.7149
XY= 0.5380 YY= 27.6280 ZY= 0.2725
XZ= 2.1799 YZ= -0.1898 ZZ= 26.8193
Eigenvalues: 26.1141 27.6260 29.8474
36 H Isotropic = 27.0927 Anisotropy = 7.1063
XX= 31.5970 YX= -0.4756 ZX= -0.1615
XY= -0.7871 YY= 23.6052 ZY= -1.7529
XZ= -2.0608 YZ= -0.7949 ZZ= 26.0759
Eigenvalues: 22.9447 26.5031 31.8302
37 H Isotropic = 27.9657 Anisotropy = 6.2753
XX= 30.7795 YX= 2.0958 ZX= 1.1690
XY= 3.2559 YY= 26.8878 ZY= -0.5533
XZ= -0.1100 YZ= -0.6312 ZZ= 26.2299
Eigenvalues: 25.0308 26.7171 32.1493
38 H Isotropic = 28.0713 Anisotropy = 6.2036
XX= 28.1768 YX= 1.7017 ZX= 3.6420
XY= 2.9289 YY= 27.8127 ZY= 0.1779
XZ= 3.5217 YZ= -1.1632 ZZ= 28.2243
Eigenvalues: 23.6253 28.3815 32.2070
39 H Isotropic = 28.0354 Anisotropy = 3.9217
XX= 25.5382 YX= 0.6282 ZX= -0.3884
XY= -0.9318 YY= 28.4525 ZY= 1.1789
XZ= -0.1621 YZ= 0.9392 ZZ= 30.1157
Eigenvalues: 25.5188 27.9376 30.6499
40 H Isotropic = 30.3470 Anisotropy = 18.1599
XX= 26.3773 YX= -1.1314 ZX= -5.0627
XY= 0.4499 YY= 30.5559 ZY= 8.4691
XZ= -5.9260 YZ= 8.8372 ZZ= 34.1079
Eigenvalues: 21.0956 27.4919 42.4536
41 H Isotropic = 30.3044 Anisotropy = 15.2563
XX= 28.2479 YX= -6.0779 ZX= -6.6436
XY= -6.0784 YY= 32.5739 ZY= 2.4595
XZ= -6.8167 YZ= 2.2680 ZZ= 30.0915
Eigenvalues: 21.3520 29.0860 40.4753
42 H Isotropic = 29.9279 Anisotropy = 15.7243
XX= 39.2066 YX= 0.0925 ZX= 3.6886
XY= 0.6068 YY= 25.8711 ZY= 3.8462
XZ= 4.4376 YZ= 4.5286 ZZ= 24.7061
Eigenvalues: 20.6052 28.7678 40.4108
43 H Isotropic = 27.8588 Anisotropy = 10.0259
XX= 26.7351 YX= 2.9131 ZX= 3.9356
XY= 1.3850 YY= 31.4434 ZY= 3.3207
XZ= 2.6498 YZ= 3.6872 ZZ= 25.3977
Eigenvalues: 22.4392 26.5944 34.5427
44 H Isotropic = 28.0389 Anisotropy = 8.1778

XX= 29.9222 YX= 3.5876 ZX= -2.4668
XY= 2.3158 YY= 28.6274 ZY= -2.6907
XZ= -0.6182 YZ= -3.1426 ZZ= 25.5672
Eigenvalues: 23.7940 26.8319 33.4908
45 H Isotropic = 28.0578 Anisotropy = 22.8591
XX= 31.8119 YX= 9.3300 ZX= -3.7229
XY= 8.7624 YY= 27.5034 ZY= -9.3263
XZ= -4.9209 YZ= -8.0106 ZZ= 24.8583
Eigenvalues: 16.7240 24.1522 43.2973

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1 C Isotropic = 105.8606 Anisotropy = 25.9380
XX= 91.1967 YX= 13.0639 ZX= 7.4622
XY= 8.5414 YY= 109.1631 ZY= 11.8686
XZ= 3.0024 YZ= -0.9214 ZZ= 117.2220
Eigenvalues: 85.9326 108.4966 123.1526
2 C Isotropic = 115.2730 Anisotropy = 39.3268
XX= 102.3193 YX= 6.1355 ZX= 8.2745
XY= 6.2806 YY= 114.8727 ZY= 22.3080
XZ= 3.8057 YZ= 10.7564 ZZ= 128.6269
Eigenvalues: 99.7252 104.6029 141.4908
3 C Isotropic = 107.5341 Anisotropy = 22.2557
XX= 112.4294 YX= 5.0530 ZX= -2.7130
XY= 12.4264 YY= 99.6046 ZY= -4.7332
XZ= -6.8350 YZ= -10.8275 ZZ= 110.5682
Eigenvalues: 93.5866 106.6445 122.3712
4 C Isotropic = 112.0499 Anisotropy = 30.3617
XX= 106.9482 YX= -0.0453 ZX= 11.3204
XY= -7.1571 YY= 112.7124 ZY= -17.6814
XZ= 13.3681 YZ= -6.1343 ZZ= 116.4892
Eigenvalues: 97.1383 106.7205 132.2911
5 C Isotropic = 93.1714 Anisotropy = 39.0471
XX= 94.7367 YX= -8.5190 ZX= -9.8543
XY= -11.1472 YY= 87.9602 ZY= -21.6669
XZ= 3.9730 YZ= -29.7383 ZZ= 96.8173
Eigenvalues: 63.4468 96.8646 119.2028
6 O Isotropic = 218.2895 Anisotropy = 81.5327
XX= 217.1597 YX= -45.2346 ZX= -10.3619
XY= -35.9955 YY= 232.0235 ZY= -18.7562
XZ= 1.7959 YZ= -41.3898 ZZ= 205.6854
Eigenvalues: 168.0722 214.1517 272.6447
7 O Isotropic = 218.2269 Anisotropy = 50.3830
XX= 218.8056 YX= 7.6061 ZX= 4.8861
XY= -47.3573 YY= 231.4050 ZY= -11.2259
XZ= 5.5627 YZ= -22.1196 ZZ= 204.4701
Eigenvalues: 195.4502 207.4150 251.8156
8 C Isotropic = 83.6730 Anisotropy = 20.3991
XX= 86.6322 YX= 1.1219 ZX= 7.7423
XY= 7.0675 YY= 95.6713 ZY= -2.4169
XZ= 7.8693 YZ= -5.1123 ZZ= 68.7155
Eigenvalues: 64.9829 88.7637 97.2724
9 O Isotropic = 296.1993 Anisotropy = 68.3492
XX= 334.8494 YX= -26.7111 ZX= 13.0345
XY= -19.8257 YY= 263.0142 ZY= -3.3528

XZ= -14.7843 YZ= -12.2858 ZZ= 290.7344
Eigenvalues: 254.4797 292.3528 341.7654
10 O Isotropic = 292.6901 Anisotropy = 37.2187
XX= 279.6631 YX= 0.7359 ZX= -21.6211
XY= 15.0132 YY= 315.1537 ZY= 19.1101
XZ= -7.1235 YZ= -4.0849 ZZ= 283.2536
Eigenvalues: 264.6331 295.9348 317.5026
11 C Isotropic = 122.4169 Anisotropy = 51.3918
XX= 136.6367 YX= 12.3978 ZX= -18.9724
XY= 13.3285 YY= 115.6680 ZY= -21.2261
XZ= -13.6217 YZ= -18.9388 ZZ= 114.9459
Eigenvalues: 95.0018 115.5707 156.6781
12 O Isotropic = 296.3892 Anisotropy = 46.9204
XX= 318.1794 YX= 10.8908 ZX= -9.0314
XY= -24.9846 YY= 277.4887 ZY= -18.2113
XZ= -24.0312 YZ= -37.4208 ZZ= 293.4994
Eigenvalues: 252.7663 308.7317 327.6694
13 O Isotropic = 294.6976 Anisotropy = 24.6249
XX= 301.6053 YX= -2.1686 ZX= 1.5671
XY= -10.3584 YY= 289.2264 ZY= -8.5030
XZ= 17.8574 YZ= -2.4432 ZZ= 293.2612
Eigenvalues: 285.3749 287.6038 311.1142
14 C Isotropic = 100.1168 Anisotropy = 27.3021
XX= 84.8579 YX= 1.4105 ZX= -10.5853
XY= 6.9104 YY= 117.2223 ZY= 0.0213
XZ= -3.8402 YZ= -4.7701 ZZ= 98.2703
Eigenvalues: 81.4808 100.5515 118.3182
15 C Isotropic = 110.0611 Anisotropy = 39.5047
XX= 109.4249 YX= 4.4242 ZX= -14.4680
XY= -2.1155 YY= 110.9594 ZY= -7.6578
XZ= -32.6443 YZ= -15.0642 ZZ= 109.7991
Eigenvalues: 84.0193 109.7666 136.3976
16 C Isotropic = 103.4001 Anisotropy = 51.8555
XX= 100.0793 YX= 9.9902 ZX= -32.9539
XY= -1.7185 YY= 95.6334 ZY= -11.4333
XZ= -21.7470 YZ= -7.6309 ZZ= 114.4876
Eigenvalues: 78.5768 93.6531 137.9704
17 O Isotropic = 234.1693 Anisotropy = 105.6904
XX= 181.4600 YX= -14.3198 ZX= -11.6656
XY= -10.6827 YY= 303.2231 ZY= -3.5047
XZ= -22.2933 YZ= -6.7614 ZZ= 217.8247
Eigenvalues: 173.3587 224.5196 304.6296
18 C Isotropic = 118.9989 Anisotropy = 49.6650
XX= 101.6012 YX= 11.2746 ZX= -0.1651
XY= 6.5869 YY= 146.4728 ZY= -11.4544
XZ= -1.2298 YZ= -14.7692 ZZ= 108.9228
Eigenvalues: 99.3665 105.5212 152.1089
19 O Isotropic = 300.0625 Anisotropy = 39.3008
XX= 315.9473 YX= 5.4371 ZX= -13.2673
XY= -18.3587 YY= 293.3041 ZY= 34.0776
XZ= 9.4150 YZ= 27.1019 ZZ= 290.9359
Eigenvalues: 261.3306 312.5938 326.2630
20 O Isotropic = 302.2998 Anisotropy = 99.3817
XX= 278.1475 YX= -21.4923 ZX= 31.6512
XY= -0.4352 YY= 283.5539 ZY= -23.8617

XZ= 20.2745 YZ= -42.7901 ZZ= 345.1981
Eigenvalues: 268.7828 269.5624 368.5543
21 O Isotropic = 296.2197 Anisotropy = 57.8592
XX= 330.0262 YX= 15.1044 ZX= 16.5214
XY= 2.6229 YY= 296.6827 ZY= 8.2086
XZ= 13.8354 YZ= -18.6183 ZZ= 261.9502
Eigenvalues: 257.4682 296.3983 334.7925
22 C Isotropic = 125.5903 Anisotropy = 56.2326
XX= 153.8597 YX= 5.1265 ZX= 23.9812
XY= 5.8099 YY= 114.0149 ZY= 3.7599
XZ= 18.5711 YZ= 1.5142 ZZ= 108.8962
Eigenvalues: 100.4107 113.2815 163.0787
23 O Isotropic = 306.2306 Anisotropy = 51.6489
XX= 287.9495 YX= 9.2687 ZX= -7.7420
XY= 41.7208 YY= 321.9420 ZY= -4.8765
XZ= -8.9366 YZ= -14.9996 ZZ= 308.8004
Eigenvalues: 274.0840 303.9446 340.6632
24 H Isotropic = 27.7447 Anisotropy = 3.7676
XX= 28.0362 YX= 1.6696 ZX= 1.8939
XY= -0.1823 YY= 26.1538 ZY= 0.0356
XZ= 0.9780 YZ= 1.0930 ZZ= 29.0443
Eigenvalues: 25.8937 27.0840 30.2565
25 H Isotropic = 28.4959 Anisotropy = 2.6433
XX= 29.6267 YX= -0.4032 ZX= 0.4595
XY= -1.8809 YY= 27.7197 ZY= 0.8076
XZ= 0.0365 YZ= 2.0429 ZZ= 28.1411
Eigenvalues: 26.1755 29.0541 30.2580
26 H Isotropic = 28.1731 Anisotropy = 8.3149
XX= 31.9847 YX= 2.6487 ZX= -0.8729
XY= 3.7691 YY= 27.6361 ZY= -0.1773
XZ= -0.6432 YZ= 0.8539 ZZ= 24.8985
Eigenvalues: 24.5589 26.2441 33.7164
27 H Isotropic = 28.3950 Anisotropy = 3.9988
XX= 29.0595 YX= -2.0340 ZX= -1.3333
XY= -2.8357 YY= 27.1065 ZY= 0.3659
XZ= -1.0848 YZ= -1.0266 ZZ= 29.0189
Eigenvalues: 25.2141 28.9100 31.0608
28 H Isotropic = 26.3794 Anisotropy = 2.7671
XX= 27.1166 YX= -0.9757 ZX= -1.1199
XY= -0.0283 YY= 25.1006 ZY= 0.9071
XZ= -0.2439 YZ= 1.6735 ZZ= 26.9210
Eigenvalues: 24.4248 26.4894 28.2241
29 H Isotropic = 28.2879 Anisotropy = 23.9462
XX= 43.8253 YX= -2.9071 ZX= 0.3002
XY= -3.2590 YY= 20.7577 ZY= -4.4700
XZ= 0.0236 YZ= -3.9947 ZZ= 20.2807
Eigenvalues: 16.1322 24.4794 44.2520
30 H Isotropic = 29.8582 Anisotropy = 18.1292
XX= 27.6653 YX= 10.9416 ZX= 1.2337
XY= 11.2251 YY= 33.3336 ZY= -1.5321
XZ= 0.2698 YZ= -0.2794 ZZ= 28.5756
Eigenvalues: 18.9226 28.7076 41.9443
31 H Isotropic = 27.6967 Anisotropy = 5.8983
XX= 27.7364 YX= 4.3914 ZX= 3.3235
XY= 3.9018 YY= 26.6079 ZY= -1.0674

XZ= 1.8389 YZ= -2.7499 ZZ= 28.7460
Eigenvalues: 21.6018 29.8595 31.6289
 32 H Isotropic = 28.1726 Anisotropy = 5.7526
XX= 31.3085 YX= -2.6557 ZX= -1.2040
XY= -0.8154 YY= 27.6793 ZY= -2.7141
XZ= -0.8292 YZ= -1.6938 ZZ= 25.5299
Eigenvalues: 23.7247 28.7853 32.0077
 33 H Isotropic = 29.8289 Anisotropy = 17.5514
XX= 25.4660 YX= 1.9177 ZX= 3.0355
XY= 2.9450 YY= 32.6092 ZY= -9.6383
XZ= 4.2313 YZ= -9.2952 ZZ= 31.4115
Eigenvalues: 19.4305 28.5263 41.5298
 34 H Isotropic = 27.4493 Anisotropy = 26.4215
XX= 26.5144 YX= 9.9753 ZX= 10.5175
XY= 9.9428 YY= 24.1332 ZY= 6.0989
XZ= 8.6543 YZ= 6.5032 ZZ= 31.7003
Eigenvalues: 15.0300 22.2542 45.0636
 35 H Isotropic = 27.8097 Anisotropy = 3.5249
XX= 29.3816 YX= -1.0845 ZX= 0.7881
XY= 0.1987 YY= 27.1467 ZY= 0.4266
XZ= 2.3138 YZ= -0.0198 ZZ= 26.9008
Eigenvalues: 26.0268 27.2426 30.1596
 36 H Isotropic = 27.1609 Anisotropy = 7.0671
XX= 31.6740 YX= -0.3976 ZX= -0.0193
XY= -0.5872 YY= 23.7840 ZY= -1.8552
XZ= -2.0922 YZ= -0.8864 ZZ= 26.0247
Eigenvalues: 23.0390 26.5713 31.8723
 37 H Isotropic = 28.0493 Anisotropy = 6.3915
XX= 30.7812 YX= 2.1862 ZX= 1.2743
XY= 3.4100 YY= 27.1149 ZY= -0.5658
XZ= 0.0822 YZ= -0.6024 ZZ= 26.2518
Eigenvalues: 25.0258 26.8118 32.3103
 38 H Isotropic = 28.0265 Anisotropy = 5.7320
XX= 28.4643 YX= 1.6078 ZX= 3.5681
XY= 3.1051 YY= 27.8184 ZY= -0.4588
XZ= 2.9849 YZ= -1.2085 ZZ= 27.7969
Eigenvalues: 23.6309 28.6008 31.8479
 39 H Isotropic = 27.7504 Anisotropy = 3.6085
XX= 24.7526 YX= 0.7704 ZX= -0.5503
XY= -1.2622 YY= 29.0710 ZY= 0.9551
XZ= -0.1759 YZ= 0.7510 ZZ= 29.4275
Eigenvalues: 24.7168 28.3782 30.1561
 40 H Isotropic = 30.2770 Anisotropy = 17.9646
XX= 26.1016 YX= -1.1234 ZX= -5.2896
XY= 0.5938 YY= 30.6238 ZY= 8.1747
XZ= -6.1093 YZ= 8.5310 ZZ= 34.1057
Eigenvalues: 20.9942 27.5835 42.2534
 41 H Isotropic = 31.2998 Anisotropy = 21.8337
XX= 24.0300 YX= -0.8621 ZX= 5.3464
XY= -1.5106 YY= 30.5763 ZY= -8.9760
XZ= 5.4803 YZ= -8.2590 ZZ= 39.2931
Eigenvalues: 21.8534 26.1904 45.8556
 42 H Isotropic = 30.0143 Anisotropy = 16.4241
XX= 40.5741 YX= 1.3214 ZX= 1.1670
XY= 1.5401 YY= 25.6608 ZY= 4.0933

XZ= 2.0221 YZ= 4.8670 ZZ= 23.8080
Eigenvalues: 20.1539 28.9253 40.9637
43 H Isotropic = 27.8867 Anisotropy = 10.0208
XX= 26.7397 YX= 2.6880 ZX= 3.9659
XY= 1.2370 YY= 31.2553 ZY= 3.6280
XZ= 2.5916 YZ= 3.9432 ZZ= 25.6651
Eigenvalues: 22.4826 26.6104 34.5672
44 H Isotropic = 28.0502 Anisotropy = 8.1526
XX= 29.7201 YX= 3.6866 ZX= -2.3294
XY= 2.3378 YY= 29.0269 ZY= -2.5639
XZ= -0.5269 YZ= -3.0113 ZZ= 25.4036
Eigenvalues: 23.8827 26.7826 33.4852
45 H Isotropic = 28.1049 Anisotropy = 22.7394
XX= 30.9991 YX= 9.3824 ZX= -3.0744
XY= 8.8144 YY= 29.0505 ZY= -9.4369
XZ= -4.3101 YZ= -8.1965 ZZ= 24.2651
Eigenvalues: 16.8110 24.2392 43.2645

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1 C Isotropic = 105.9387 Anisotropy = 30.1562
XX= 116.8985 YX= 11.1493 ZX= -16.0293
XY= 0.4332 YY= 108.9133 ZY= -0.0803
XZ= -11.3284 YZ= -9.6318 ZZ= 92.0042
Eigenvalues: 85.7542 106.0190 126.0428
2 C Isotropic = 114.6831 Anisotropy = 37.9365
XX= 122.9641 YX= 16.9089 ZX= -15.5561
XY= 7.4537 YY= 112.4966 ZY= -5.3612
XZ= -13.8562 YZ= -11.0011 ZZ= 108.5885
Eigenvalues: 99.3711 104.7040 139.9741
3 C Isotropic = 108.7738 Anisotropy = 23.1203
XX= 112.2416 YX= -2.5514 ZX= 10.0363
XY= -10.8057 YY= 115.6672 ZY= -5.6928
XZ= 5.4062 YZ= -5.6213 ZZ= 98.4126
Eigenvalues: 94.6257 107.5084 124.1873
4 C Isotropic = 112.1236 Anisotropy = 31.2191
XX= 108.3458 YX= 0.7477 ZX= -0.8431
XY= 11.9326 YY= 125.4413 ZY= 10.0635
XZ= 4.5384 YZ= 15.5968 ZZ= 102.5836
Eigenvalues: 96.7505 106.6839 132.9363
5 C Isotropic = 91.0676 Anisotropy = 34.6719
XX= 71.7500 YX= -9.3089 ZX= 16.2549
XY= -1.6817 YY= 110.9464 ZY= 16.2081
XZ= 12.2136 YZ= 1.2930 ZZ= 90.5064
Eigenvalues: 62.3932 96.6274 114.1822
6 O Isotropic = 222.0766 Anisotropy = 81.1355
XX= 173.3132 YX= -0.7608 ZX= 22.0064
XY= -9.6763 YY= 237.9797 ZY= 39.5111
XZ= 2.0896 YZ= 16.5411 ZZ= 254.9371
Eigenvalues: 170.1553 219.9076 276.1670
7 O Isotropic = 217.1639 Anisotropy = 38.4068
XX= 198.8546 YX= -3.6002 ZX= -13.6301
XY= -13.6502 YY= 220.7800 ZY= 18.0065
XZ= 21.9145 YZ= 12.8446 ZZ= 231.8571
Eigenvalues: 193.4116 215.3117 242.7685

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  8  C    Isotropic =    77.3312   Anisotropy =    36.0120
XX=    87.3841   YX=   -17.5577   ZX=    -1.4119
XY=   -21.0120   YY=    66.5645   ZY=     7.8967
XZ=    -1.8556   YZ=    14.9891   ZZ=    78.0450
Eigenvalues:    51.8375    78.8168   101.3392
  9  O    Isotropic =   297.3958   Anisotropy =    70.6466
XX=   283.5168   YX=    25.5625   ZX=    35.8288
XY=    -1.6305   YY=   290.9476   ZY=    -5.1046
XZ=    42.3179   YZ=     8.6062   ZZ=   317.7230
Eigenvalues:   255.5979   292.0960   344.4935
 10  O    Isotropic =   292.4459   Anisotropy =    36.4767
XX=   294.9341   YX=   -13.2615   ZX=    -7.7169
XY=   -22.3241   YY=   284.3008   ZY=     5.5479
XZ=   -27.0623   YZ=   -15.3101   ZZ=   298.1030
Eigenvalues:   264.4264   296.1477   316.7637
 11  C    Isotropic =   121.2437   Anisotropy =    51.9036
XX=   121.6730   YX=   -27.3507   ZX=    17.0555
XY=   -22.0219   YY=   133.7222   ZY=    -1.3887
XZ=    14.6065   YZ=    -1.9986   ZZ=   108.3361
Eigenvalues:    92.7104   115.1746   155.8462
 12  O    Isotropic =   297.4839   Anisotropy =    46.9044
XX=   277.5383   YX=    -8.6478   ZX=    12.1539
XY=   -17.6715   YY=   314.4813   ZY=     7.2556
XZ=    50.6957   YZ=   -10.9509   ZZ=   300.4321
Eigenvalues:   253.9478   309.7504   328.7535
 13  O    Isotropic =   301.0132   Anisotropy =    16.6056
XX=   302.7780   YX=    -6.2128   ZX=     9.1798
XY=    10.5812   YY=   303.7505   ZY=     8.8823
XZ=    11.6572   YZ=    -2.7165   ZZ=   296.5111
Eigenvalues:   288.6704   302.2856   312.0836
 14  C    Isotropic =   104.1304   Anisotropy =    24.9920
XX=   117.2468   YX=     1.2570   ZX=   -17.7789
XY=     4.3365   YY=   100.4517   ZY=    -7.5933
XZ=     0.7442   YZ=     0.8166   ZZ=    94.6927
Eigenvalues:    91.2205   100.3791   120.7917
 15  C    Isotropic =   104.7985   Anisotropy =    27.3996
XX=   121.6909   YX=     1.3890   ZX=    11.9161
XY=     8.7687   YY=    95.0862   ZY=     7.2747
XZ=    -5.2700   YZ=    -6.5193   ZZ=    97.6184
Eigenvalues:    94.1324    97.1982   123.0649
 16  C    Isotropic =    92.4327   Anisotropy =    34.5098
XX=    81.3429   YX=    -9.8890   ZX=    12.0661
XY=   -24.1597   YY=    97.4653   ZY=    -0.2394
XZ=    14.8454   YZ=    -7.3251   ZZ=    98.4899
Eigenvalues:    67.4863    94.3725   115.4392
 17  O    Isotropic =   225.0508   Anisotropy =   126.7855
XX=   224.2042   YX=   -69.6601   ZX=   -13.8616
XY=   -62.5672   YY=   207.4336   ZY=    36.6279
XZ=   -31.8120   YZ=    38.5254   ZZ=   243.5148
Eigenvalues:   147.1190   218.4590   309.5745
 18  C    Isotropic =   120.8233   Anisotropy =    51.1085
XX=   121.5382   YX=   -19.6259   ZX=   -14.3870
XY=   -21.2202   YY=   130.6626   ZY=    15.2564
XZ=   -10.5942   YZ=    12.7417   ZZ=   110.2690
Eigenvalues:   102.1272   105.4470   154.8956
```

19 O Isotropic = 272.1205 Anisotropy = 108.9543
XX= 325.1499 YX= -13.9423 ZX= -11.0430
XY= -33.3680 YY= 242.7224 ZY= 37.2398
XZ= -40.4901 YZ= 36.0346 ZZ= 248.4894
Eigenvalues: 208.8552 262.7497 344.7567
20 O Isotropic = 302.2594 Anisotropy = 92.0250
XX= 276.1794 YX= 29.8346 ZX= 5.6992
XY= 7.8851 YY= 357.4446 ZY= 14.9390
XZ= -2.8987 YZ= 11.9956 ZZ= 273.1543
Eigenvalues: 270.0054 273.1635 363.6095
21 O Isotropic = 291.9950 Anisotropy = 72.0004
XX= 306.2277 YX= -27.0133 ZX= 19.9504
XY= -23.5858 YY= 279.7557 ZY= -21.3157
XZ= 26.7791 YZ= -18.4136 ZZ= 290.0015
Eigenvalues: 262.4509 273.5387 339.9953
22 C Isotropic = 123.6621 Anisotropy = 46.8754
XX= 105.3106 YX= 8.6338 ZX= 13.0202
XY= 5.8454 YY= 114.6050 ZY= 3.0122
XZ= 6.8097 YZ= 11.1808 ZZ= 151.0708
Eigenvalues: 100.7112 115.3628 154.9124
23 O Isotropic = 293.2083 Anisotropy = 25.8719
XX= 291.0288 YX= -3.9108 ZX= -13.6830
XY= -8.2790 YY= 308.2161 ZY= -9.2334
XZ= 3.5163 YZ= -0.0975 ZZ= 280.3800
Eigenvalues: 276.9090 292.2597 310.4563
24 H Isotropic = 27.7493 Anisotropy = 4.0891
XX= 29.1693 YX= 1.4563 ZX= -0.7676
XY= 2.4194 YY= 27.5675 ZY= -0.8870
XZ= 1.1178 YZ= -0.3528 ZZ= 26.5112
Eigenvalues: 25.7638 27.0088 30.4754
25 H Isotropic = 28.5178 Anisotropy = 2.3980
XX= 28.4163 YX= 0.6085 ZX= -0.3215
XY= 1.6439 YY= 27.1166 ZY= -0.5380
XZ= 1.1292 YZ= 0.0212 ZZ= 30.0205
Eigenvalues: 26.4156 29.0213 30.1165
26 H Isotropic = 28.1108 Anisotropy = 8.3811
XX= 32.2643 YX= -2.6700 ZX= 2.6274
XY= -2.2128 YY= 25.1938 ZY= -1.3238
XZ= 1.3454 YZ= -0.3268 ZZ= 26.8741
Eigenvalues: 24.4127 26.2215 33.6982
27 H Isotropic = 28.3857 Anisotropy = 3.8317
XX= 25.4769 YX= 0.8956 ZX= 0.9218
XY= 0.4588 YY= 29.0007 ZY= 0.4441
XZ= 1.3997 YZ= -1.0546 ZZ= 30.6796
Eigenvalues: 25.0946 29.1223 30.9402
28 H Isotropic = 26.2487 Anisotropy = 2.2723
XX= 25.9401 YX= 0.7003 ZX= 1.1906
XY= 1.4308 YY= 25.4601 ZY= -1.1152
XZ= -0.2443 YZ= -0.8457 ZZ= 27.3460
Eigenvalues: 24.2423 26.7404 27.7636
29 H Isotropic = 28.2170 Anisotropy = 24.5578
XX= 29.4998 YX= -0.5591 ZX= 13.6192
XY= -0.2301 YY= 23.5620 ZY= 2.7776
XZ= 14.0061 YZ= 3.4113 ZZ= 31.5892
Eigenvalues: 15.9280 24.1342 44.5889

30 H Isotropic = 29.8772 Anisotropy = 18.1117
XX= 39.3412 YX= -5.2167 ZX= -3.1301
XY= -4.9852 YY= 30.6318 ZY= -1.6171
XZ= -2.9041 YZ= -0.0887 ZZ= 19.6585
Eigenvalues: 18.9629 28.7169 41.9516
31 H Isotropic = 27.6447 Anisotropy = 5.7270
XX= 31.4515 YX= 1.0474 ZX= -0.1391
XY= -0.9832 YY= 29.9023 ZY= 1.3543
XZ= 0.7256 YZ= 0.5831 ZZ= 21.5805
Eigenvalues: 21.4609 30.0106 31.4627
32 H Isotropic = 28.1818 Anisotropy = 5.7154
XX= 26.6443 YX= -2.2747 ZX= 4.1608
XY= -1.7794 YY= 27.9366 ZY= 0.7002
XZ= 2.4248 YZ= 1.7883 ZZ= 29.9645
Eigenvalues: 23.3763 29.1771 31.9920
33 H Isotropic = 29.7937 Anisotropy = 17.5006
XX= 28.7969 YX= -2.1260 ZX= 0.9229
XY= -1.4220 YY= 39.5807 ZY= 5.8322
XZ= -0.6045 YZ= 5.7665 ZZ= 21.0035
Eigenvalues: 19.2978 28.6226 41.4608
34 H Isotropic = 27.3230 Anisotropy = 25.5945
XX= 41.8445 YX= 7.2562 ZX= -2.5121
XY= 6.3435 YY= 24.7012 ZY= -1.0306
XZ= -1.8657 YZ= 0.0330 ZZ= 15.4234
Eigenvalues: 15.2428 22.3403 44.3860
35 H Isotropic = 27.2628 Anisotropy = 4.9797
XX= 26.1387 YX= 1.4285 ZX= 1.2989
XY= 1.7733 YY= 27.7988 ZY= 2.6999
XZ= 0.6913 YZ= 1.2895 ZZ= 27.8510
Eigenvalues: 25.1399 26.0660 30.5826
36 H Isotropic = 27.5875 Anisotropy = 5.2567
XX= 27.6909 YX= 1.1214 ZX= 2.3871
XY= 0.9258 YY= 27.4280 ZY= -3.2957
XZ= 3.3430 YZ= -2.1559 ZZ= 27.6438
Eigenvalues: 23.0976 28.5730 31.0920
37 H Isotropic = 27.7987 Anisotropy = 8.0812
XX= 31.3170 YX= -2.9184 ZX= -0.2846
XY= -3.4213 YY= 27.7299 ZY= 1.1937
XZ= 0.4778 YZ= 0.8207 ZZ= 24.3491
Eigenvalues: 23.9030 26.3068 33.1861
38 H Isotropic = 27.9861 Anisotropy = 5.5301
XX= 31.5416 YX= 1.2767 ZX= 1.0299
XY= -0.6554 YY= 28.9151 ZY= 0.2857
XZ= 0.5625 YZ= 1.1461 ZZ= 23.5016
Eigenvalues: 23.3398 28.9457 31.6728
39 H Isotropic = 27.7838 Anisotropy = 3.1272
XX= 26.7875 YX= -0.0968 ZX= -2.7998
XY= 0.4845 YY= 28.3927 ZY= -0.2539
XZ= -1.2353 YZ= -0.9767 ZZ= 28.1711
Eigenvalues: 25.3330 28.1497 29.8686
40 H Isotropic = 31.6350 Anisotropy = 19.4654
XX= 43.1744 YX= -5.6535 ZX= 0.1807
XY= -3.9805 YY= 27.9593 ZY= 1.7040
XZ= -0.6318 YZ= 3.3050 ZZ= 23.7711
Eigenvalues: 22.4114 27.8815 44.6119

41 H Isotropic = 31.1972 Anisotropy = 22.0036
XX= 25.9919 YX= 3.0561 ZX= -0.6729
XY= 3.7023 YY= 44.3185 ZY= 4.5756
XZ= -0.4221 YZ= 4.9840 ZZ= 23.2812
Eigenvalues: 21.8273 25.8980 45.8662
42 H Isotropic = 29.4786 Anisotropy = 18.4664
XX= 36.6347 YX= -1.0469 ZX= 6.9738
XY= -1.6383 YY= 21.0290 ZY= -4.9861
XZ= 6.3053 YZ= -5.7428 ZZ= 30.7722
Eigenvalues: 18.5134 28.1330 41.7895
43 H Isotropic = 28.5705 Anisotropy = 6.8992
XX= 25.5897 YX= -2.0399 ZX= 2.8028
XY= -1.9740 YY= 31.5715 ZY= -0.6628
XZ= 2.7601 YZ= -1.7839 ZZ= 28.5504
Eigenvalues: 23.7529 28.7888 33.1700
44 H Isotropic = 27.3963 Anisotropy = 5.4626
XX= 26.9424 YX= 1.0942 ZX= 1.2195
XY= 0.8477 YY= 26.4250 ZY= 2.9888
XZ= -1.6019 YZ= 3.3230 ZZ= 28.8213
Eigenvalues: 23.9683 27.1825 31.0380
45 H Isotropic = 28.5645 Anisotropy = 18.7623
XX= 28.5089 YX= -8.2649 ZX= 5.4525
XY= -9.5716 YY= 32.5571 ZY= -1.9992
XZ= 4.4431 YZ= -2.2329 ZZ= 24.6275
Eigenvalues: 19.6885 24.9323 41.0727

Sucrose_122

1 C Isotropic = 110.2035 Anisotropy = 40.7699
XX= 94.9490 YX= 12.9210 ZX= 11.4968
XY= 15.2369 YY= 115.0782 ZY= 12.9283
XZ= 13.1419 YZ= 9.4379 ZZ= 120.5832
Eigenvalues: 86.4604 106.7666 137.3834
2 C Isotropic = 116.2854 Anisotropy = 45.9079
XX= 100.3142 YX= 4.3259 ZX= 12.1887
XY= 6.9962 YY= 114.4108 ZY= 24.2410
XZ= 9.0425 YZ= 9.4402 ZZ= 134.1311
Eigenvalues: 97.1927 104.7728 146.8906
3 C Isotropic = 108.4296 Anisotropy = 22.7708
XX= 113.5696 YX= 5.6313 ZX= -2.0424
XY= 13.8740 YY= 102.2343 ZY= -5.5742
XZ= -5.5161 YZ= -11.6767 ZZ= 109.4849
Eigenvalues: 94.2124 107.4662 123.6102
4 C Isotropic = 111.8233 Anisotropy = 30.1701
XX= 107.7741 YX= -0.6878 ZX= 12.4734
XY= -6.9264 YY= 112.1854 ZY= -17.0085
XZ= 13.1887 YZ= -6.0845 ZZ= 115.5104
Eigenvalues: 96.8573 106.6759 131.9367
5 C Isotropic = 91.3635 Anisotropy = 37.2652
XX= 93.8539 YX= -9.9417 ZX= -9.1337
XY= -11.7112 YY= 86.9005 ZY= -20.8100
XZ= 3.0666 YZ= -28.6229 ZZ= 93.3360
Eigenvalues: 61.9292 95.9542 116.2069
6 O Isotropic = 221.1557 Anisotropy = 61.8384
XX= 221.3187 YX= -16.0286 ZX= -17.0032

XY= -16.0450 YY= 237.8382 ZY= -23.6246
XZ= -2.7915 YZ= -47.9161 ZZ= 204.3101
Eigenvalues: 175.2239 225.8618 262.3813
7 O Isotropic = 215.8499 Anisotropy = 45.3255
XX= 219.9873 YX= 11.6349 ZX= 6.6006
XY= -36.9803 YY= 223.2690 ZY= -19.6115
XZ= 9.9322 YZ= -23.4041 ZZ= 204.2934
Eigenvalues: 190.2736 211.2091 246.0669
8 C Isotropic = 83.0982 Anisotropy = 22.9191
XX= 86.3583 YX= 5.0828 ZX= 8.4715
XY= 9.1643 YY= 94.0666 ZY= -3.3241
XZ= 10.7061 YZ= -5.2526 ZZ= 68.8696
Eigenvalues: 63.1022 87.8148 98.3776
9 O Isotropic = 298.5893 Anisotropy = 71.3659
XX= 338.8623 YX= -28.9300 ZX= 16.1068
XY= -19.4769 YY= 265.6542 ZY= -2.4581
XZ= -17.8146 YZ= -11.4613 ZZ= 291.2513
Eigenvalues: 256.9816 292.6197 346.1665
10 O Isotropic = 298.1786 Anisotropy = 36.8860
XX= 289.9924 YX= 10.7093 ZX= -17.5924
XY= 17.2909 YY= 316.2819 ZY= 17.4205
XZ= -4.1998 YZ= -0.1946 ZZ= 288.2614
Eigenvalues: 272.3951 299.3714 322.7693
11 C Isotropic = 124.4401 Anisotropy = 53.1799
XX= 150.3377 YX= -19.9629 ZX= -3.6676
XY= -21.9593 YY= 112.2784 ZY= -7.1433
XZ= -9.9962 YZ= -5.8043 ZZ= 110.7042
Eigenvalues: 97.2857 116.1412 159.8934
12 O Isotropic = 297.9218 Anisotropy = 47.1172
XX= 319.6401 YX= 11.4653 ZX= -9.2123
XY= -24.4455 YY= 279.2938 ZY= -18.7048
XZ= -23.8395 YZ= -37.4309 ZZ= 294.8315
Eigenvalues: 254.3388 310.0933 329.3333
13 O Isotropic = 313.5278 Anisotropy = 67.3671
XX= 324.5177 YX= 19.3524 ZX= 8.2773
XY= 50.5223 YY= 319.8637 ZY= 5.2427
XZ= -1.1106 YZ= 12.6999 ZZ= 296.2019
Eigenvalues: 285.4398 296.7043 358.4392
14 C Isotropic = 99.2368 Anisotropy = 25.4343
XX= 83.8507 YX= 0.9323 ZX= -14.1707
XY= 8.0638 YY= 114.6438 ZY= 0.6239
XZ= -5.3477 YZ= -5.1093 ZZ= 99.2160
Eigenvalues: 78.8455 102.6720 116.1930
15 C Isotropic = 111.0073 Anisotropy = 39.9267
XX= 114.2732 YX= 3.1555 ZX= -16.4743
XY= -3.9520 YY= 110.7767 ZY= -8.4082
XZ= -32.1274 YZ= -14.0687 ZZ= 107.9720
Eigenvalues: 83.7135 111.6833 137.6251
16 C Isotropic = 101.3376 Anisotropy = 52.2982
XX= 99.6123 YX= 6.2858 ZX= -35.4041
XY= -4.9693 YY= 93.0392 ZY= -10.0716
XZ= -22.9928 YZ= -5.1935 ZZ= 111.3613
Eigenvalues: 74.6477 93.1620 136.2031
17 O Isotropic = 233.1822 Anisotropy = 103.5757
XX= 182.7574 YX= -11.7394 ZX= -8.8789

XY= -5.4966 YY= 299.9763 ZY= -11.3636
XZ= -19.5857 YZ= -14.0878 ZZ= 216.8129
Eigenvalues: 176.3225 220.9914 302.2327
 18 C Isotropic = 117.7547 Anisotropy = 47.5409
XX= 99.2337 YX= 13.2781 ZX= 3.8962
XY= 7.5508 YY= 143.6279 ZY= -11.8676
XZ= 3.4988 YZ= -13.4941 ZZ= 110.4027
Eigenvalues: 93.9825 109.8331 149.4487
 19 O Isotropic = 298.7109 Anisotropy = 40.5515
XX= 314.7516 YX= 3.3122 ZX= -7.7669
XY= -21.6575 YY= 292.9895 ZY= 35.2591
XZ= 13.3882 YZ= 30.0820 ZZ= 288.3914
Eigenvalues: 256.7416 313.6458 325.7452
 20 O Isotropic = 298.2966 Anisotropy = 52.0439
XX= 302.0425 YX= -34.4076 ZX= -16.3097
XY= -7.3652 YY= 281.5413 ZY= 3.5248
XZ= -14.6675 YZ= 21.2028 ZZ= 311.3058
Eigenvalues: 268.3727 293.5244 332.9925
 21 O Isotropic = 292.2331 Anisotropy = 53.8733
XX= 318.7338 YX= 11.7703 ZX= 26.2238
XY= 1.4563 YY= 290.2108 ZY= -0.8383
XZ= 20.9773 YZ= -19.5006 ZZ= 267.7548
Eigenvalues: 254.5401 294.0106 328.1487
 22 C Isotropic = 125.6203 Anisotropy = 52.5395
XX= 147.4606 YX= 7.8496 ZX= 26.0421
XY= 9.5885 YY= 115.2649 ZY= 2.5338
XZ= 19.5359 YZ= 0.9324 ZZ= 114.1354
Eigenvalues: 102.0824 114.1318 160.6466
 23 O Isotropic = 308.1362 Anisotropy = 53.0243
XX= 308.0554 YX= 12.8916 ZX= -8.4641
XY= 30.5488 YY= 312.6062 ZY= -8.6325
XZ= -22.0479 YZ= -20.9364 ZZ= 303.7470
Eigenvalues: 288.1100 292.8129 343.4857
 24 H Isotropic = 28.0891 Anisotropy = 4.4399
XX= 29.7560 YX= -0.0900 ZX= 2.7724
XY= -0.5258 YY= 25.7339 ZY= -0.1610
XZ= 0.6488 YZ= 1.3994 ZZ= 28.7776
Eigenvalues: 25.4987 27.7197 31.0491
 25 H Isotropic = 27.9286 Anisotropy = 2.1954
XX= 27.9670 YX= -0.7206 ZX= 1.2097
XY= -2.2264 YY= 27.7116 ZY= -0.0471
XZ= 0.2962 YZ= 0.8569 ZZ= 28.1073
Eigenvalues: 26.0411 28.3525 29.3922
 26 H Isotropic = 28.1795 Anisotropy = 8.4752
XX= 32.1869 YX= 2.4441 ZX= -0.7559
XY= 3.7802 YY= 27.8071 ZY= -0.2419
XZ= -0.7109 YZ= 0.8883 ZZ= 24.5446
Eigenvalues: 24.3106 26.3983 33.8297
 27 H Isotropic = 28.3964 Anisotropy = 3.7217
XX= 28.9995 YX= -2.2249 ZX= -1.0288
XY= -2.9621 YY= 26.8176 ZY= 0.1622
XZ= -0.8812 YZ= -1.4034 ZZ= 29.3720
Eigenvalues: 24.8513 29.4603 30.8775
 28 H Isotropic = 26.4072 Anisotropy = 2.5248
XX= 27.1414 YX= -1.4241 ZX= -0.5322

XY= -0.4703 YY= 24.9731 ZY= 0.9851
XZ= 0.2326 YZ= 1.6031 ZZ= 27.1072
Eigenvalues: 24.1470 26.9843 28.0904
29 H Isotropic = 27.9576 Anisotropy = 25.5664
XX= 44.4714 YX= -3.3113 ZX= 0.8420
XY= -3.6412 YY= 20.1427 ZY= -4.3284
XZ= 0.1166 YZ= -3.8917 ZZ= 19.2587
Eigenvalues: 15.4290 23.4419 45.0019
30 H Isotropic = 29.9537 Anisotropy = 18.4245
XX= 28.0191 YX= 10.8906 ZX= 1.8600
XY= 11.0691 YY= 33.7390 ZY= -1.5341
XZ= 1.2351 YZ= 0.1507 ZZ= 28.1029
Eigenvalues: 19.2269 28.3975 42.2367
31 H Isotropic = 27.7141 Anisotropy = 8.8108
XX= 32.9027 YX= 3.3706 ZX= 1.6986
XY= 1.1922 YY= 25.7580 ZY= -3.2498
XZ= 1.1273 YZ= -3.7539 ZZ= 24.4814
Eigenvalues: 21.0106 28.5437 33.5879
32 H Isotropic = 27.7090 Anisotropy = 5.5383
XX= 26.7636 YX= -2.0311 ZX= -1.5134
XY= -1.7475 YY= 25.1313 ZY= 0.7127
XZ= -0.0465 YZ= -0.4347 ZZ= 31.2320
Eigenvalues: 23.8759 27.8498 31.4011
33 H Isotropic = 29.6094 Anisotropy = 17.4651
XX= 25.1571 YX= 1.7519 ZX= 3.5600
XY= 2.8059 YY= 32.2053 ZY= -9.4169
XZ= 4.8419 YZ= -9.1881 ZZ= 31.4659
Eigenvalues: 19.0228 28.5526 41.2528
34 H Isotropic = 31.4285 Anisotropy = 17.0311
XX= 39.0802 YX= 4.9054 ZX= 4.4429
XY= 4.7575 YY= 31.9836 ZY= 2.0682
XZ= 5.1312 YZ= 0.9415 ZZ= 23.2217
Eigenvalues: 21.8860 29.6170 42.7825
35 H Isotropic = 27.7316 Anisotropy = 2.8883
XX= 28.9642 YX= -0.8349 ZX= 0.5764
XY= 0.5292 YY= 27.3950 ZY= 0.1822
XZ= 2.1742 YZ= -0.4811 ZZ= 26.8356
Eigenvalues: 26.1572 27.3804 29.6571
36 H Isotropic = 27.2077 Anisotropy = 7.1244
XX= 31.4615 YX= -0.7019 ZX= -0.7604
XY= -1.2063 YY= 24.1767 ZY= -1.5409
XZ= -2.4654 YZ= -0.5153 ZZ= 25.9848
Eigenvalues: 23.4052 26.2606 31.9573
37 H Isotropic = 27.9456 Anisotropy = 6.2834
XX= 30.6850 YX= 2.3171 ZX= 0.9149
XY= 3.2464 YY= 26.7940 ZY= -0.5094
XZ= -0.3988 YZ= -0.7048 ZZ= 26.3578
Eigenvalues: 25.0213 26.6810 32.1345
38 H Isotropic = 28.0582 Anisotropy = 6.3484
XX= 27.9413 YX= 1.7476 ZX= 3.6735
XY= 3.0022 YY= 27.8414 ZY= 0.4449
XZ= 3.4900 YZ= -0.8979 ZZ= 28.3918
Eigenvalues: 23.6678 28.2164 32.2904
39 H Isotropic = 27.9677 Anisotropy = 3.8242
XX= 25.8095 YX= 0.4570 ZX= -0.3315

XY= -1.0117 YY= 28.1872 ZY= 1.2605
XZ= -0.1396 YZ= 1.0659 ZZ= 29.9066
Eigenvalues: 25.7747 27.6114 30.5172
40 H Isotropic = 30.4851 Anisotropy = 18.2729
XX= 27.1056 YX= -1.5874 ZX= -5.3606
XY= 0.0421 YY= 30.9848 ZY= 8.6607
XZ= -6.2776 YZ= 8.9797 ZZ= 33.3649
Eigenvalues: 21.0871 27.7012 42.6671
41 H Isotropic = 29.9448 Anisotropy = 15.4357
XX= 27.7824 YX= -5.8906 ZX= -7.2089
XY= -5.9516 YY= 31.3959 ZY= 2.2740
XZ= -7.3904 YZ= 2.0854 ZZ= 30.6562
Eigenvalues: 20.6380 28.9611 40.2353
42 H Isotropic = 30.0954 Anisotropy = 15.4607
XX= 38.8460 YX= -0.1001 ZX= 4.3162
XY= 0.4840 YY= 26.3183 ZY= 3.7969
XZ= 4.9327 YZ= 4.3713 ZZ= 25.1217
Eigenvalues: 20.9152 28.9684 40.4025
43 H Isotropic = 27.8741 Anisotropy = 9.4814
XX= 26.2755 YX= 2.6246 ZX= 3.5321
XY= 1.0476 YY= 31.8495 ZY= 2.8406
XZ= 2.3463 YZ= 3.4397 ZZ= 25.4972
Eigenvalues: 22.7364 26.6907 34.1950
44 H Isotropic = 28.2497 Anisotropy = 8.5531
XX= 30.0850 YX= 3.7813 ZX= -2.3353
XY= 2.5441 YY= 28.7344 ZY= -3.2041
XZ= -0.4812 YZ= -3.3811 ZZ= 25.9297
Eigenvalues: 23.6856 27.1118 33.9518
45 H Isotropic = 28.4069 Anisotropy = 25.1094
XX= 35.2550 YX= 9.6090 ZX= -5.2244
XY= 9.0035 YY= 24.7098 ZY= -9.2678
XZ= -6.3364 YZ= -7.6323 ZZ= 25.2560
Eigenvalues: 15.9742 24.1001 45.1466

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