

# Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A

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## Supplemental Information

### Table of Contents

|   |    |
|---|----|
| Supplemental Information .....  | 1  |
| General Experimental Procedures .....   | 2  |
| NMR Data Acquisition.....   | 2  |
| Rationale for the contradictory results of C-7 configuration by Mosher analysis in the previous works ..... | 6  |
| Residual Chemical Shift Anisotropy data acquisition .....   | 9  |
| Overview of Phormidolide A Structure Revision .....   | 13 |
| DP4 Epimeric C7 isomers of Phormidolide A Fragments .....   | 14 |
| Revised Phormidolide A Structure and Diastereomeric Fragments utilized.....                                 | 15 |
| Scalar Coupling Constants and <sup>13</sup> C Chemical Shifts Analysis.....                                 | 16 |
| SVD Analysis of Diastereomeric Phormidolide A Fragments .....   | 16 |
| Conformer Generation and Computation .....  | 17 |
| DFT Structures of the seven conformations of Phormidolide A ( <i>SRS</i> ) .....                            | 19 |
| Chemical Shielding Tensors of the seven conformations of Phormidolide A ( <i>SRS</i> ) .....                | 26 |
| Conformer 1.....  | 26 |
| Conformer 2.....  | 34 |
| Conformer 3.....  | 41 |
| Conformer 4.....  | 49 |
| Conformer 5.....  | 57 |
| Conformer 6.....  | 65 |
| Conformer 7.....  | 73 |
| References .....  | 82 |

## General Experimental Procedures

HPLC was done using a semi-preparative column coupled to a Thermo Dionex Ultimate 3000 pump, RS autosampler, RS diode array detector, and automated fraction collector.

**Culture Conditions:** ISB3NOV94-8A was initially collected in Sulawesi, Indonesia and kept in culture in SWBG11 media. It was grown in 16 hour light / 8 hour dark routine at 27-28°C for approximately 90 days before harvest.

**Extraction and Isolation:** Multiple harvests of the culture were combined and extracted in DCM/MeOH (2:1) to afford a crude of 1.8724g. The crude was fractionated by Vacuum Liquid Chromatography, and Fraction H (75:25 EtOAc/MeOH) had phormidolide A present. This fraction was put on semi-preparative HPLC with a Kinetex 5  $\mu$ m C18 150 x 10.0 mm semi-preparative column and using a linear gradient with (A) H<sub>2</sub>O to (B) CH<sub>3</sub>CN at a flow rate of 2.5 mL/min from 30% to 99% (B) ( $t_R$ =26.5-30.7 min). This fraction was further purified using an isocratic method (60:35:5 EtOAc/hexanes/IPA) at 4.5 mL/min on Preparative HPLC with a Luna 5  $\mu$ m Silica 250 x 10.00 mm semi-preparative column to yield 12 mg of pure phormidolide A.

## NMR Data Acquisition

Approximately 5 mg of the phormidolide A sample was dissolved in 500  $\mu$ L CDCl<sub>3</sub> solvent with 5  $\mu$ L of TMS added as internal reference and the mixture vortex before being transferred into a 5 mm NMR tube. Isotropic NMR data was acquired as follows; <sup>1</sup>H NMR experiment (9090.9 Hz spectral width, 32,768 t1 points and 2 total scans), <sup>13</sup>C NMR experiment (35,714.3 Hz spectral width, 32,768 t1 points and 492 total scans), COSY experiment (5882.4\*5882.4 F1\*F2 spectral width, 2048\*256 t2\*t1 points with a total of 2 scans), HSQC experiment (5882.4\*23041 F1\*F2 spectral width, 1024\*384 t2\*t1 points, 4 scans) and HSQC\_TOCSY experiment (5882.4\*23041 F1\*F2 spectral width, 1024\*384 t2\*t1 points, 12 scans). All experiments were acquired with a Bruker Avance III 600 MHz spectrometer equipped with a 5 mm TXO cryogenic probe at a probe temperature of 25 °C.

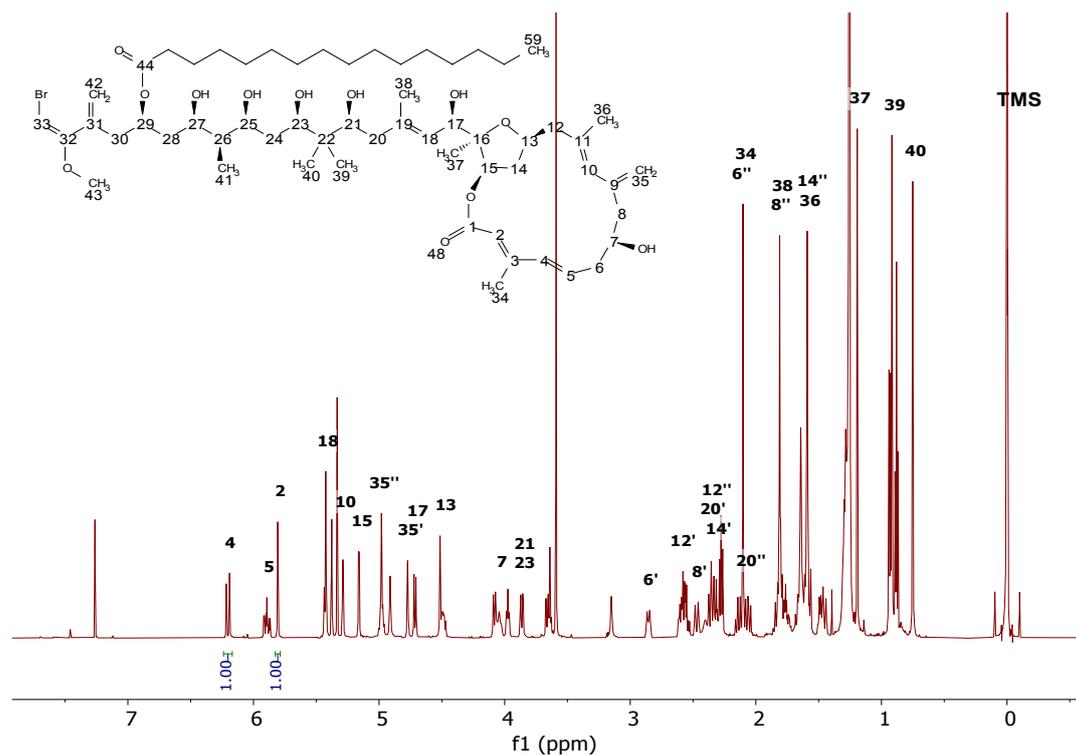


Figure S 1: Isotropic  $^1\text{H}$  NMR spectrum of phormidolide A (shown inset) in  $\text{CDCl}_3$ , showing the corresponding peaks of interest utilized for the structure revision studies presented in this work. The fully assigned chemical shift table can be found in the original reference<sup>1</sup>.

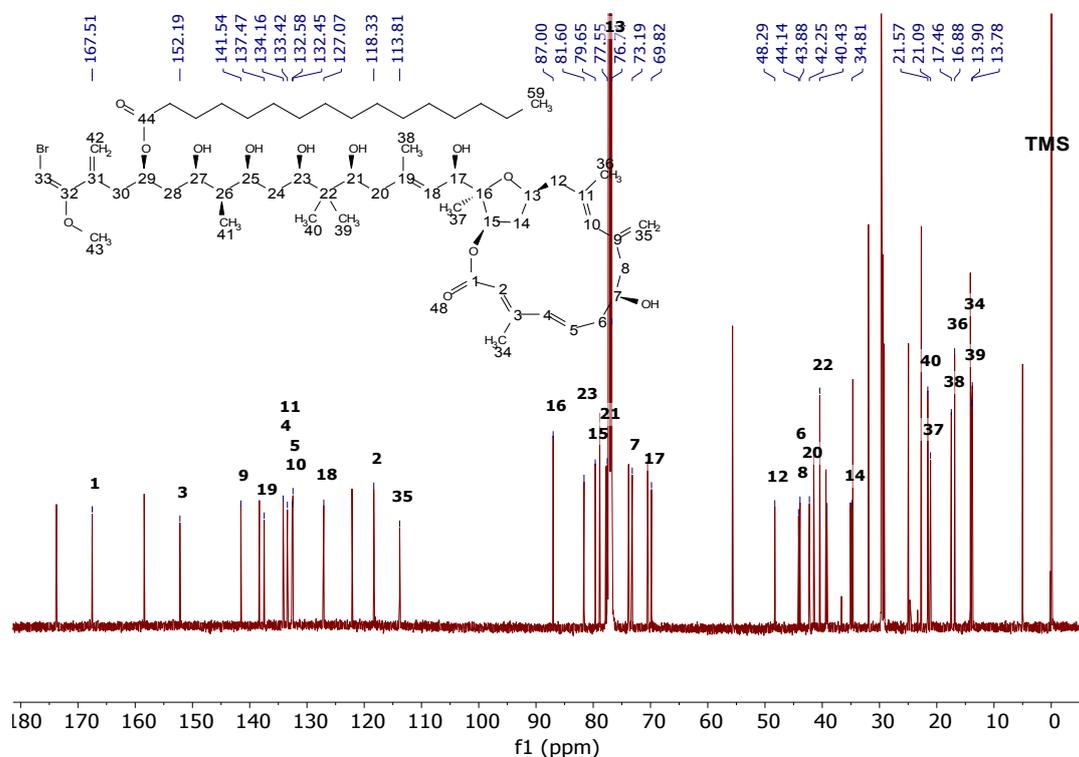


Figure S 2: Isotropic  $^{13}\text{C}$  NMR spectrum of phormidolide A (shown inset) in  $\text{CDCl}_3$ , showing the corresponding peaks of interest utilized for the structure revision studies presented in this work. The fully assigned chemical shift table can be found in the original reference<sup>1</sup>.

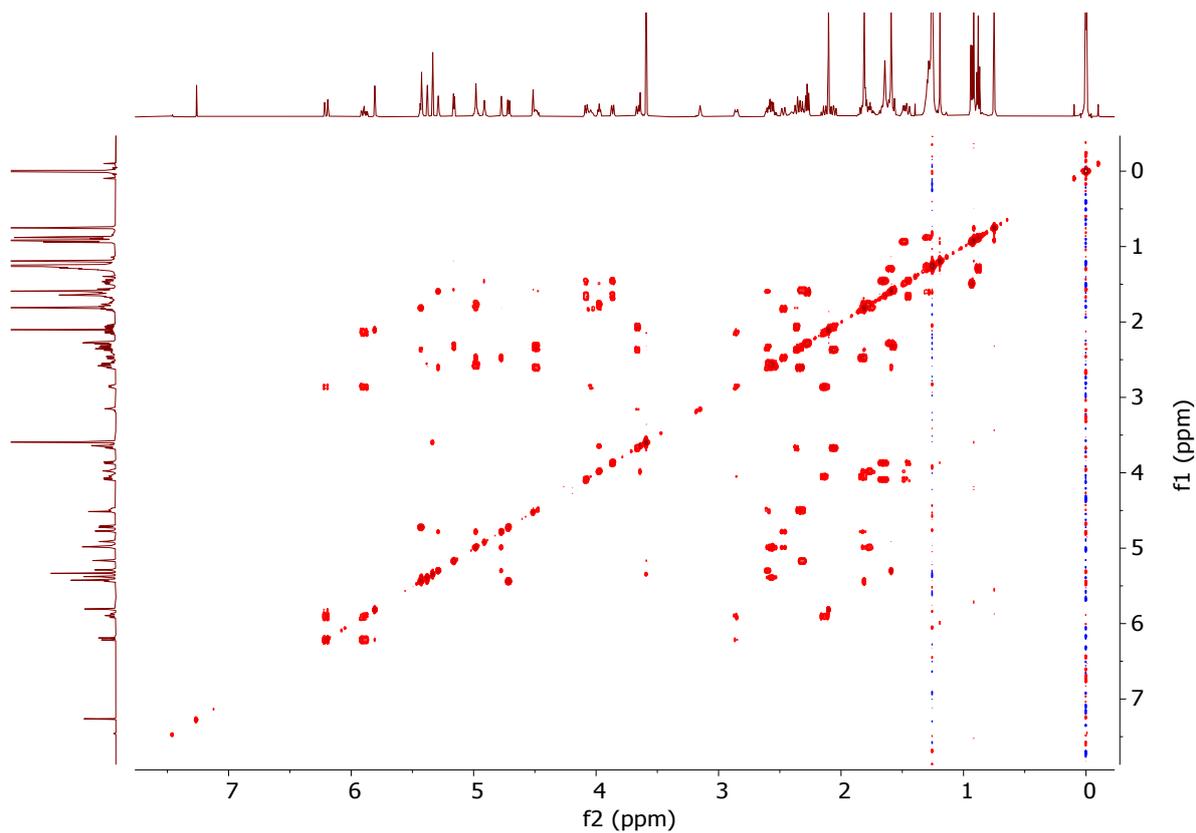


Figure S 3: COSY NMR spectrum of phormidolide A in  $\text{CDCl}_3$ . F1 and F2 traces are  $^1\text{H}$  NMR one-dimensional spectra.

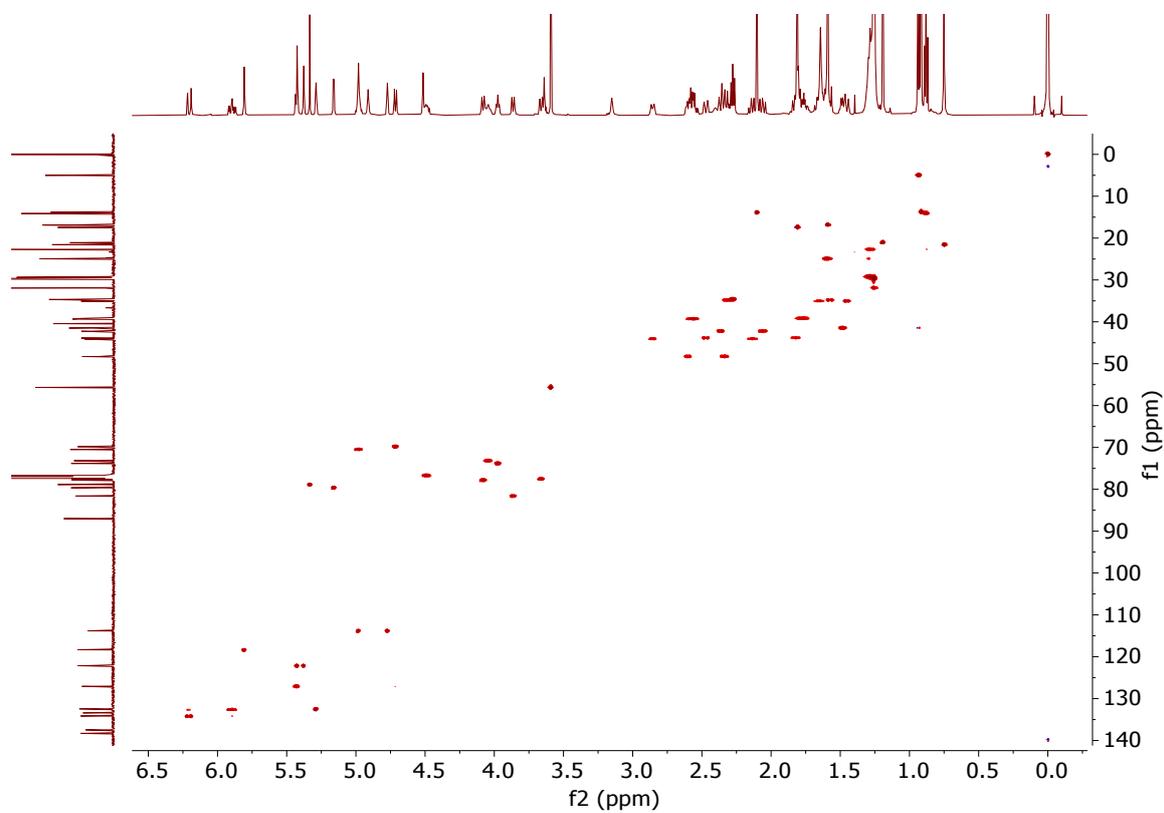


Figure S 4: HSQC NMR spectrum of phormidolide A in  $\text{CDCl}_3$ . F1 and F2 traces are, respectively,  $^1\text{H}$  and  $^{13}\text{C}$  NMR one-dimensional spectra.

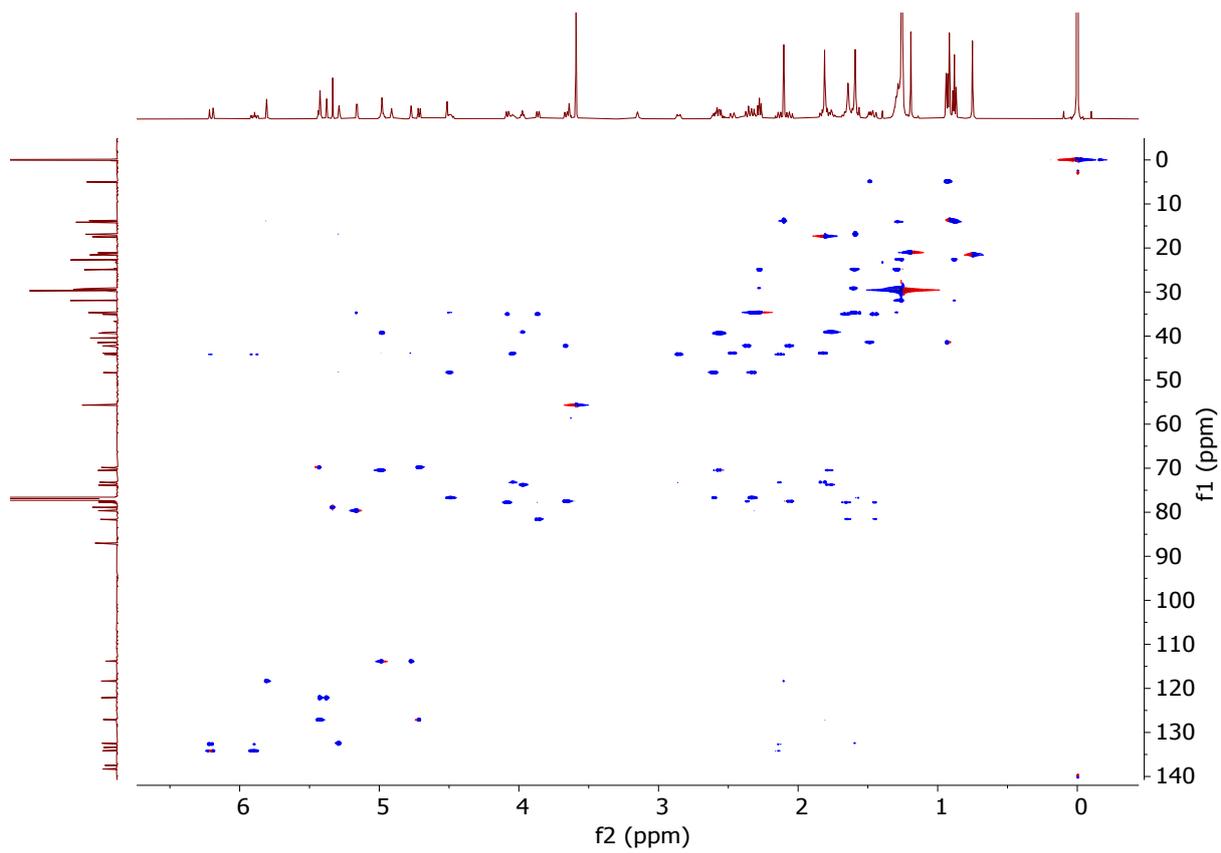
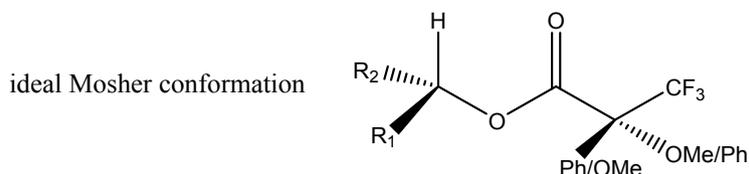


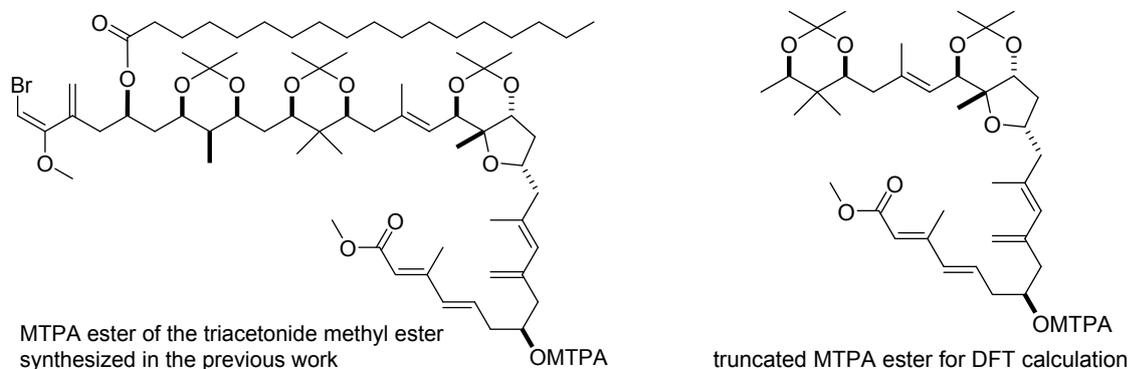
Figure S 5: HSQC-TOCSY NMR spectrum of phormidolide A in  $\text{CDCl}_3$ . F1 and F2 traces are, respectively,  $^1\text{H}$  and  $^{13}\text{C}$  NMR one-dimensional spectra

## Rationale for the contradictory results of C-7 configuration by Mosher analysis in previous work

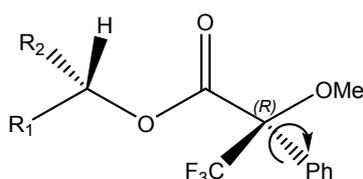
The Mosher MTPA ester analysis was established based on the assumption that, in the predominant conformer, both the  $\text{CF}_3$  group of MTPA and the  $\alpha$ -proton of the chiral alcohol are *syn*-planar with the carbonyl group as shown below.<sup>2,3</sup>



To verify the conformation of the Mosher esters synthesized in previous work, DFT calculation of the truncated MTPA ester of the linear triacetone methyl ester was carried out (conformational search was performed by MacroModel and the DFT calculation were performed at the SMD-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) level). The DFT calculations revealed that the MTPA region is highly sterically hindered, and the steric hindrance significantly twisted the MTPA conformation from the ideal conformation that Mosher analysis relies on, especially in the case of the (*R*)-MTPA ester. Therefore, the shielding pattern and  $\Delta\delta$  obtained in the previous works was highly deviated from the ideal Mosher model, resulting in incorrect C-7 assignment in the previous works.



In (*R*)-MTPA, there was no dominant conformer. The lowest energy conformer only has 9% population. In most low energy conformers, the -OMe of the MTPA aligned *syn*-planarly with the carbonyl group, and some of them had C-Ph bond rotation up to  $90^\circ$ .



In (*S*)-MTPA, there was a dominant conformer (65%). The -OMe of the MTPA aligned *anti*-planarly with the carbonyl group.

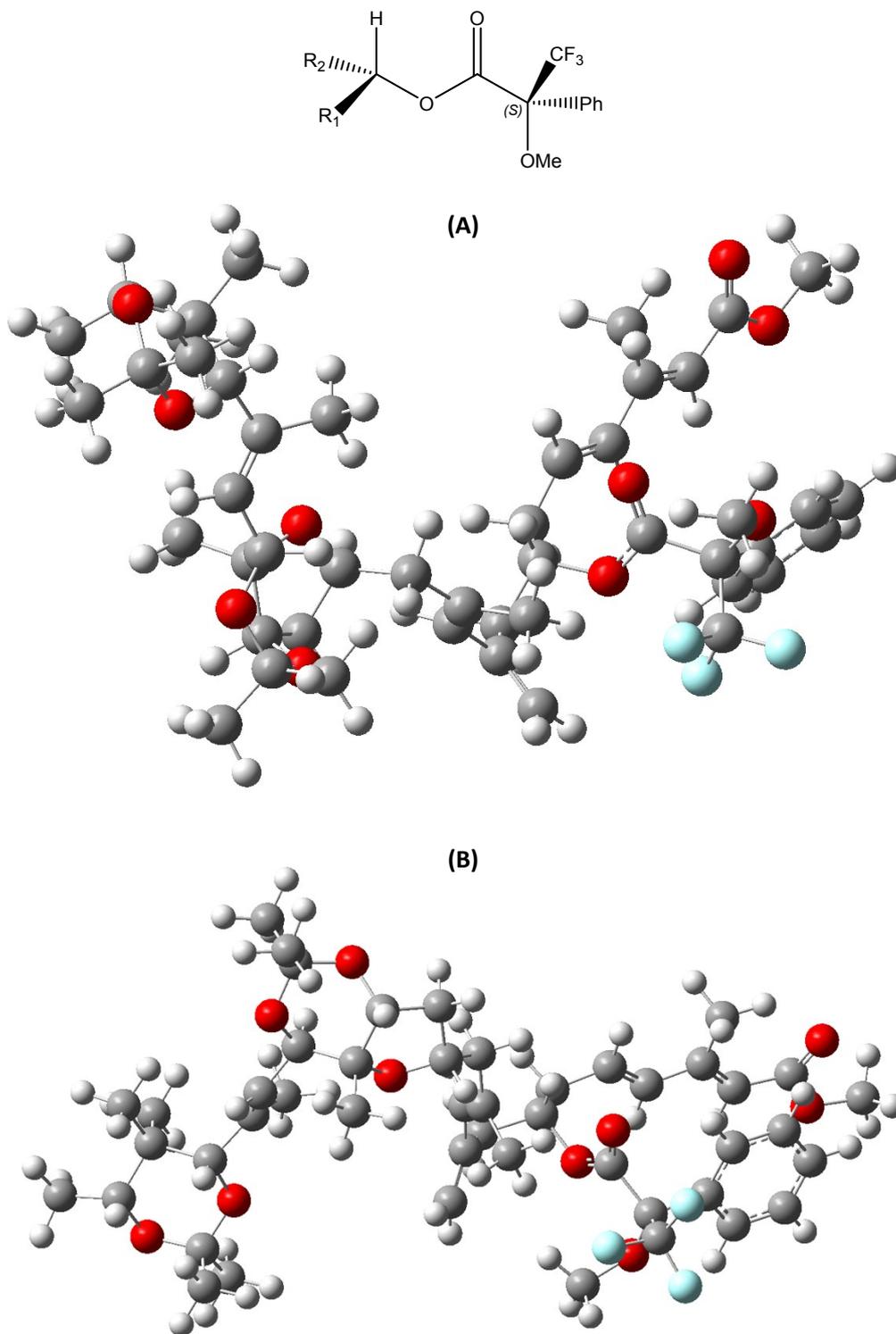
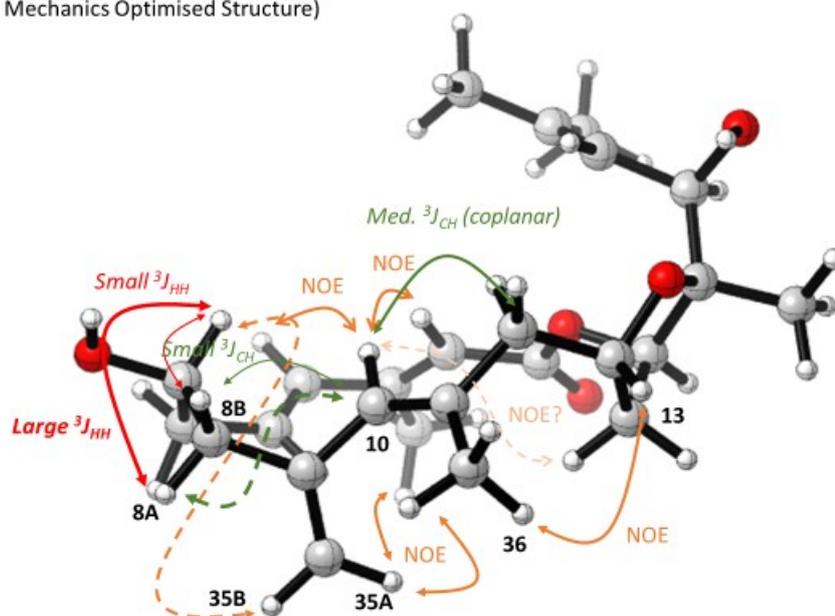


Figure S 6: (A) Conformation of the lowest energy conformer (9%) of the (*R*)-MTPA derivatives of the linear phormidolide triacetone. (B) Conformation of the lowest energy conformer (65%) of the (*S*)-MTPA derivatives of the linear phormidolide triacetone.

**7R Reported Configuration**  
(Molecular Mechanics Optimised Structure)



**7S Alternative Configuration**  
(Molecular Mechanics Optimised Structure)

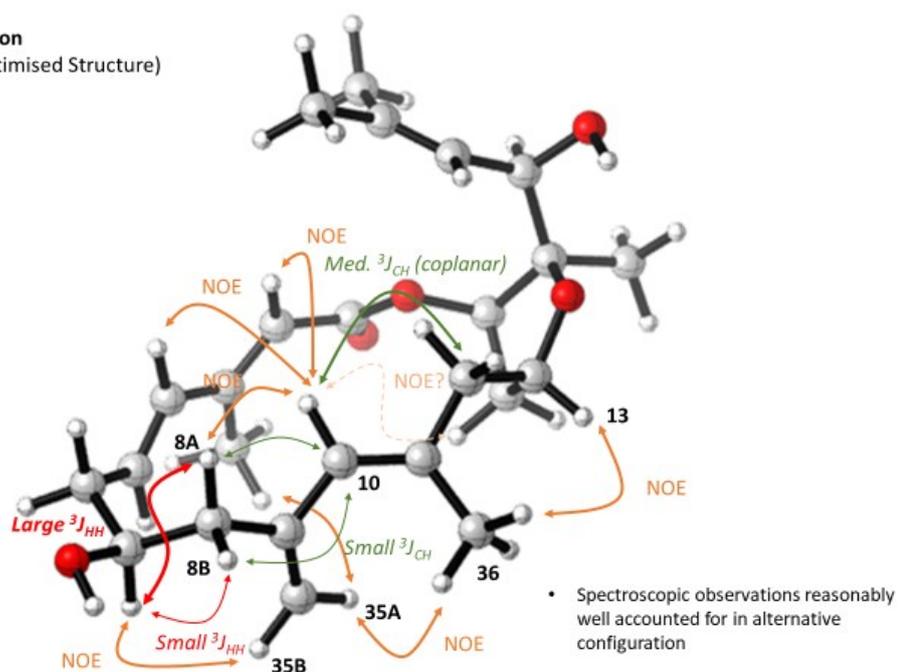


Figure S 7: MM-optimized structures for the originally reported 7R configuration and the corrected 7S configuration.

## Residual Chemical Shift Anisotropy data acquisition

Following the initial isotropic NMR data acquisition, 30.91 mg of poly- $\gamma$ -benzyl-L-glutamate (PBLG) – 150 – 300 KDa molecular weight – was added to the 500  $\mu$ L  $\text{CDCl}_3$  solution of phormidolide A contained in the NMR tube. Multiple tube inversion and spin down allowed the PBLG to fully dissolve. A second isotropic  $^{13}\text{C}$  NMR data (35,714.3 Hz spectral width, 32,768 t1 points and 808 scans) was then acquired.  $^2\text{H}$  NMR spectrum (1388.9 Hz spectral width, 4096 t1 points and 1 scan) was also acquired to confirm that the solution was still isotropic. A further 29.85 mg PBLG was added to the solution, giving a total mass concentration of 60.76 mg PBLG, followed by mixing as described earlier and then acquisition of  $^2\text{H}$  NMR spectrum (1388.9 Hz spectral width, 4096 t1 points and 1 scan) and  $^{13}\text{C}$  NMR data (35,714.3 Hz spectral width, 32,768 t1 points and 2560 scans).

Residual Chemical shift anisotropy (RCSA) data was measured using the following equation<sup>4</sup>;

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

where  $\Delta\delta_{I_0}$  is isotropic  $^{13}\text{C}$  NMR chemical shift without addition of poly- $\gamma$ -benzyl-L-glutamate (PBLG),  $\Delta\delta_{I_1}$  is isotropic  $^{13}\text{C}$  NMR chemical shift after addition of 29.85 mg of PBLG and  $\Delta\delta_{A_1}$  is anisotropic  $^{13}\text{C}$  NMR chemical shift after addition of a total 60.76 mg PBLG, which is above the solutions' PBLG critical mass concentration.  $[P]_{A_1}$  and  $[P]_{I_1}$  are mass concentrations of PBLG in the anisotropic and isotropic solutions, respectively. All  $^{13}\text{C}$  NMR spectra are referenced TMS at 0.0 ppm.

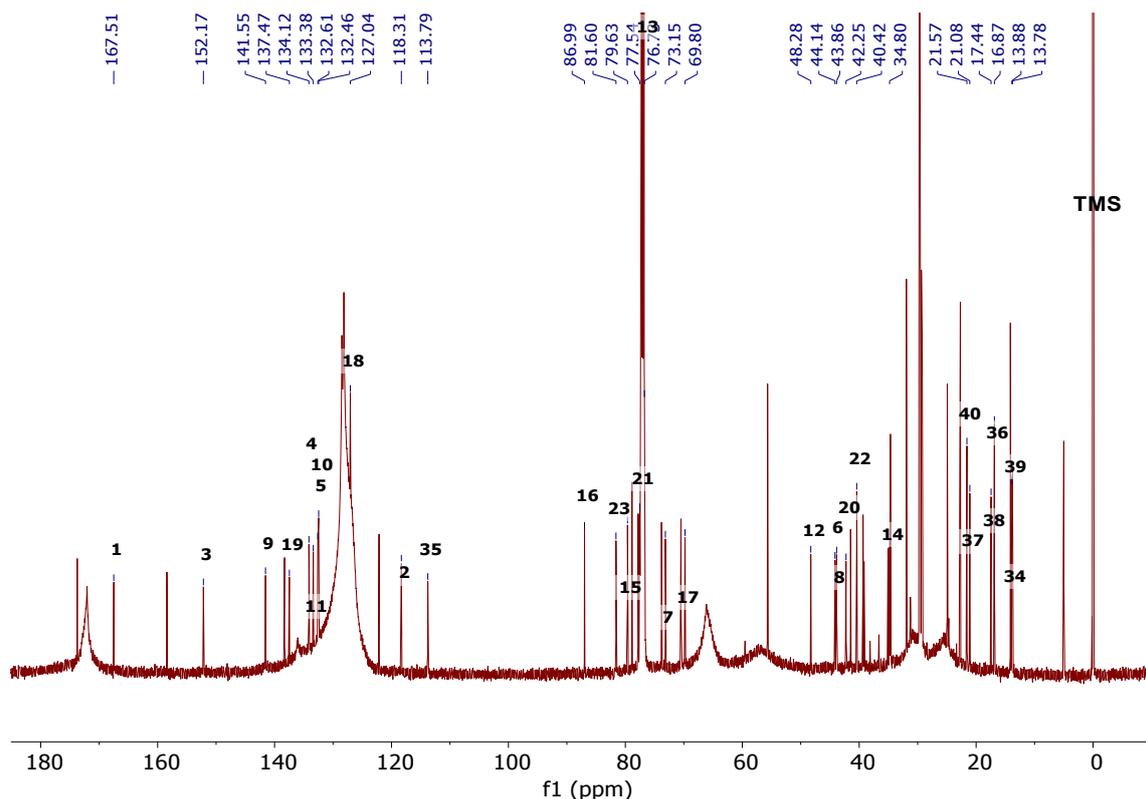


Figure S 8: Isotropic  $^{13}\text{C}$  NMR spectrum of phormidolide A in  $\text{CDCl}_3$ , after addition of 30.91 mg PBLG, showing the corresponding peaks of interest utilized for the structure revision studies presented in this work. The fully assigned chemical shift table can found in the original reference<sup>1</sup>

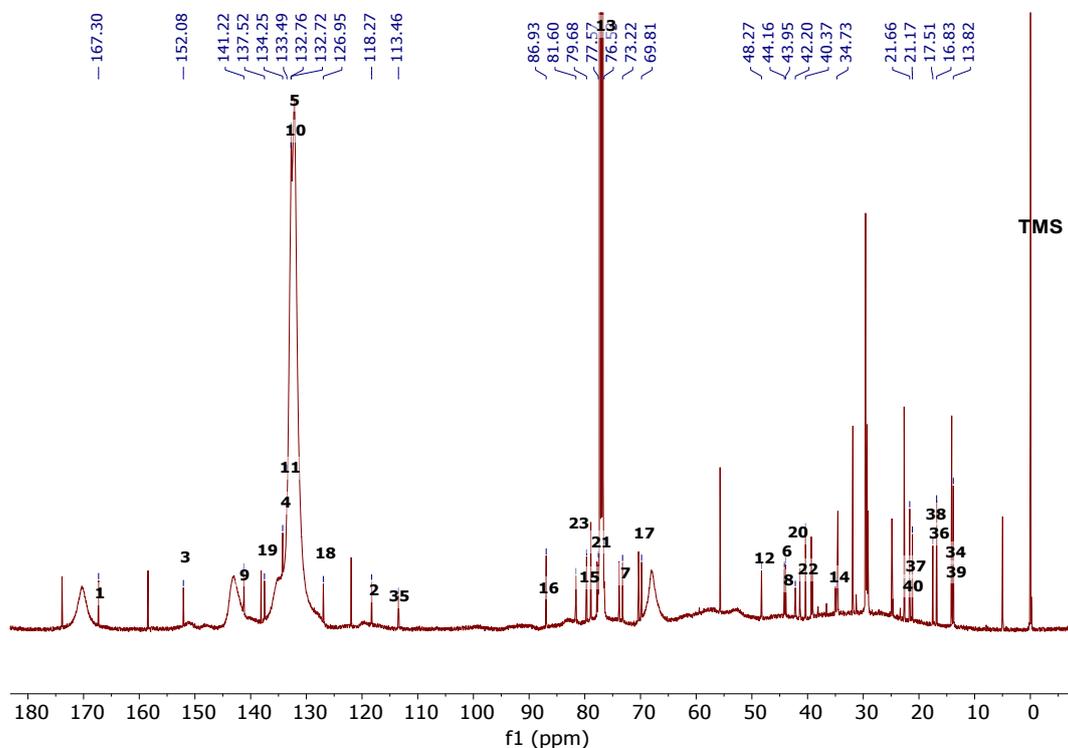


Figure S 9: Anisotropic  $^{13}\text{C}$  NMR spectrum of phormidolide A in  $\text{CDCl}_3$ , after addition of 60.76 mg PBLG, showing the corresponding peaks of interest utilized for the structure revision studies presented in this work. The fully assigned chemical shift table can found in the original reference<sup>1</sup>

Table S 1: Measured  $^{13}\text{C}$  chemical shift values (in Hz) from the isotropic and anisotropic solutions of phormidolide A sample in 500  $\mu\text{L}$   $\text{CDCl}_3$ . RCSA values are computed using the equation S1. Residual quadrupolar coupling (RQC) is also given.

| Phormidolide A Numbering   | DFT atom numbering | Isotropic $\Delta\delta_{\text{I0}}$ (Hz) | Isotropic $\Delta\delta_{\text{I1}}$ (30.91mg PBLG, Hz) | Anisotropic $\Delta\delta_{\text{A1}}$ (60.76mg PBLG, Hz) | RCSA (Hz)    |
|--|--------------------|---|---|---|--------------|
| C1   | C1                 | 25274.9                                   | 25274.2   | 25243.8   | -29.72       |
| C3   | C3                 | 22962.6                                   | 22960.3   | 22946   | -12.08       |
| C9   | C9                 | 21356.7                                   | 21357.9   | 21308.4   | -50.66       |
| C19  | C19                | 20742.5                                   | 20741.6   | 20749.6   | 8.87         |
| C4   | C4                 | 20242.3                                   | 20237.4   | 20256.1   | 23.43        |
| C11  | C11                | 20130.5                                   | 20124.7   | 20141.3   | 22.20        |
| C5   | C5                 | 20004.6                                   | 20008.7   | 20031.6   | 18.94        |
| C10  | C10                | 19984.4                                   | 19985.7   | 20025.6   | 38.64        |
| C18  | C18                | 19172.4                                   | 19168.6   | 19154.8   | -10.13       |
| C2   | C2                 | 17853.6                                   | 17851.3   | 17844.7   | -4.38        |
| C35  | C26                | 17172.5                                   | 17168.7   | 17119.1   | -45.93       |
| C16  | C16                | 13127.7                                   | 13125   | 13116.4   | -5.99        |
| C15  | C15                | 12017.7                                   | 12015   | 12022.9   | 10.51        |
| C21  | C21                | 11700.9                                   | 11700.3   | 11704.1   | 4.38         |
| C13  | C13                | 11578.8                                   | 11577.8   | 11547.9   | -28.93       |
| C7   | C7                 | 11042.6                                   | 11037.2   | 11047.5   | 15.51        |
| C17  | C17                | 10535.2                                   | 10531   | 10533.6   | 6.66         |
| C12  | C12                | 7285.5                                    | 7284.1  | 7282.7  | -0.05        |
| C6   | C6                 | 6660.3                                    | 6659.4  | 6663.6  | 5.07         |
| C8   | C8                 | 6620.9                                    | 6617.8  | 6630.9  | 16.09        |
| C20  | C20                | 6374.8                                    | 6374.6  | 6367.3  | -7.11        |
| C22  | C22                | 6100.9                                    | 6099.4  | 6090.8  | -7.15        |
| C40  | C31                | 3255                                      | 3254.8  | 3267.9  | 13.29        |
| C37  | C28                | 3182.5                                    | 3180  | 3194.9  | 17.31        |
| C38  | C29                | 2633.9                                    | 2631.2  | 2642.2  | 13.61        |
| C36  | C27                | 2546.6                                    | 2545.6  | 2538.9  | -5.73        |
| C34  | C25                | 2096.6                                    | 2094.9  | 2085.9  | -7.36        |
| C39  | C30                | 2079.7                                    | 2078.5  | 2085.9  | 8.56         |
| RQC  |                    |   |   |   | <b>266.2</b> |
| * C14 (DFT and phormidolide A numbering) signal impacted by severe line broadening |                    |   |   |   |              |

## Overview of Phormidolide A Structure Revision

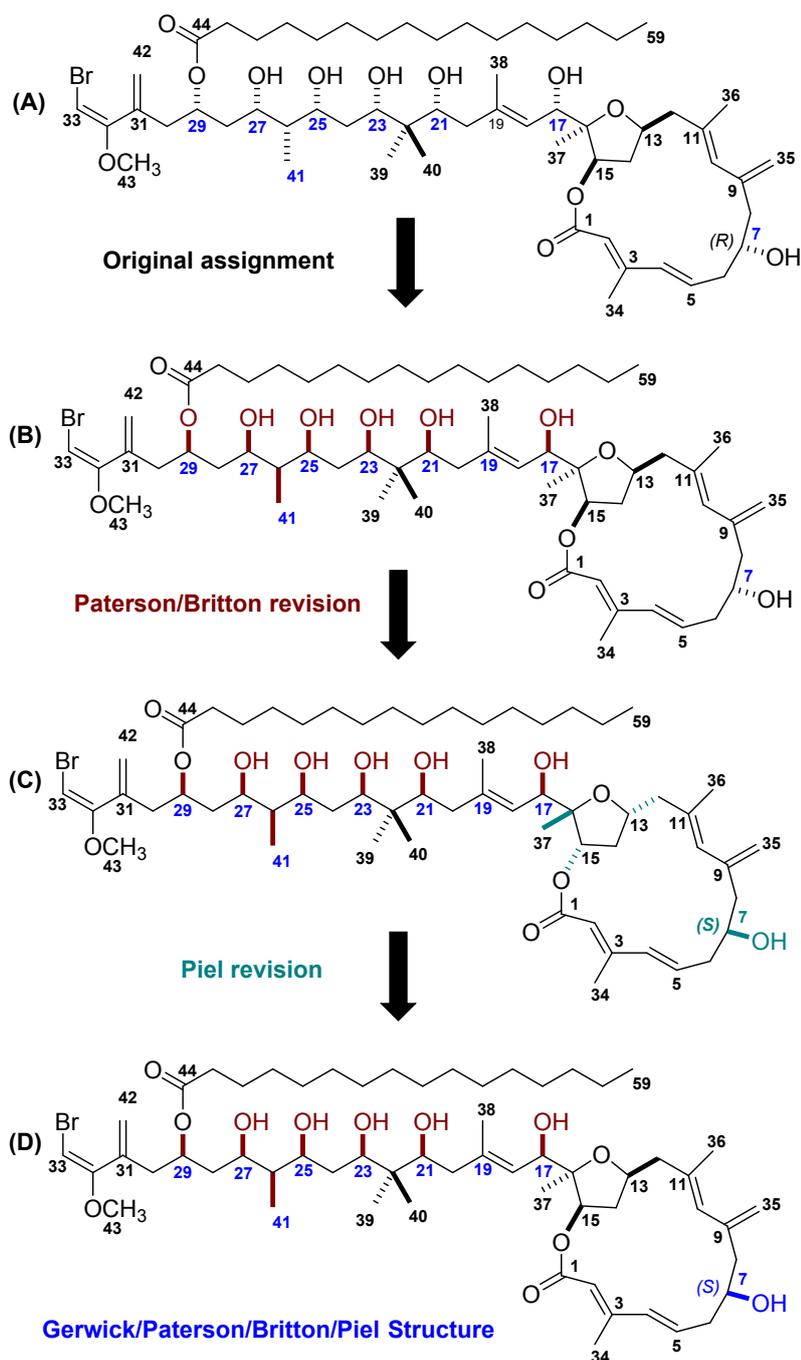


Figure S 10: Overview of phormidolide A structure reassignment strategies. (A) Original structure proposed through an extensive *J*-Based Configurational Analysis (JBCA) and Mosher ester analysis. (B) Paterson/Britton revision through synthesis and spectroscopic comparison to model diacetanides (C) Piel revision through genomic prediction and isolation of the leptolyngbyalides and (D) Gerwick/Paterson/Britton/Piel revised structure utilizing a synergistic approach, which encompasses current NMR methodologies and theoretical calculations.

## DP4 Epimeric C7 isomers of Phormidolide A Fragments

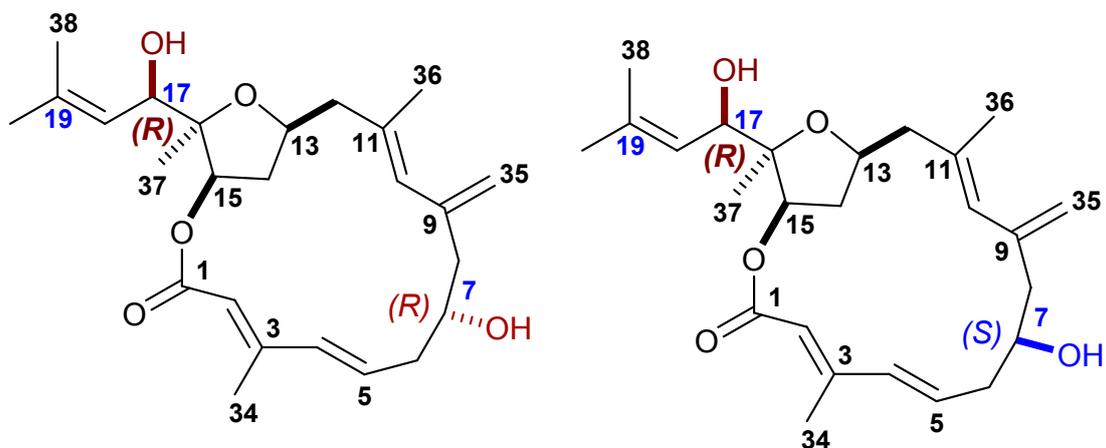
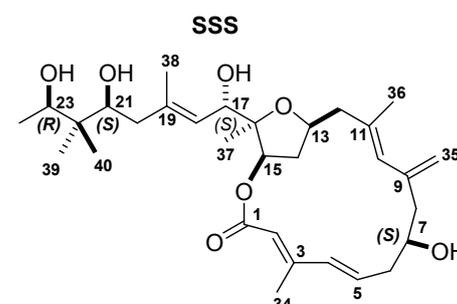
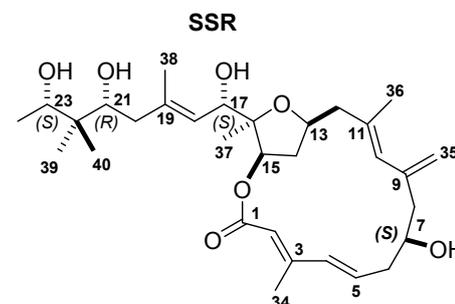
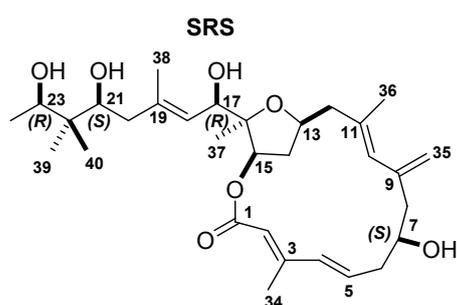
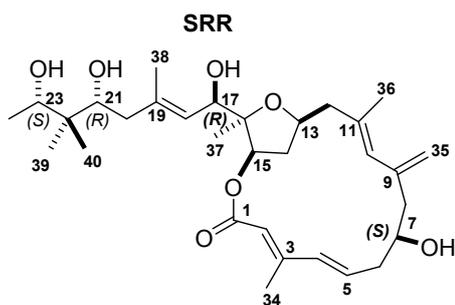
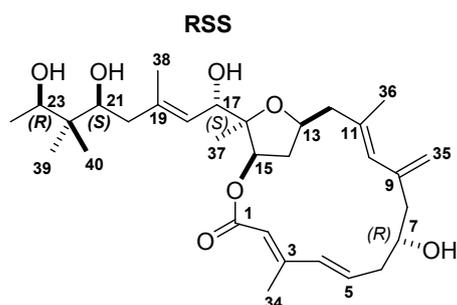
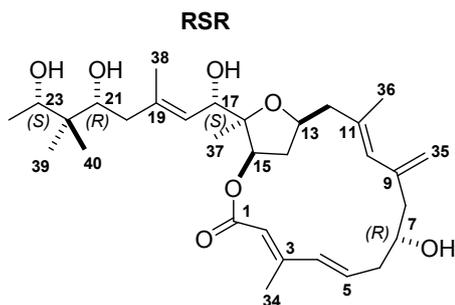
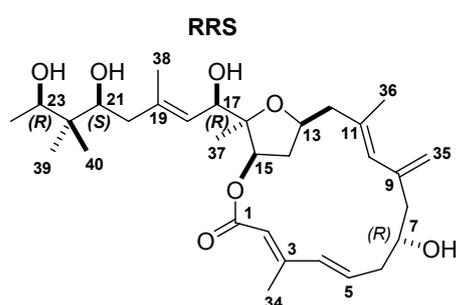
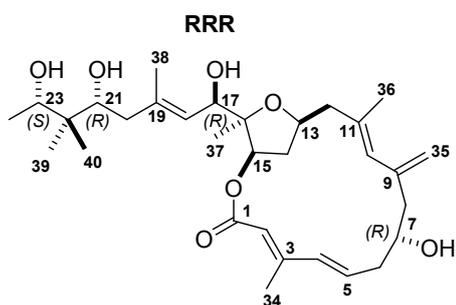
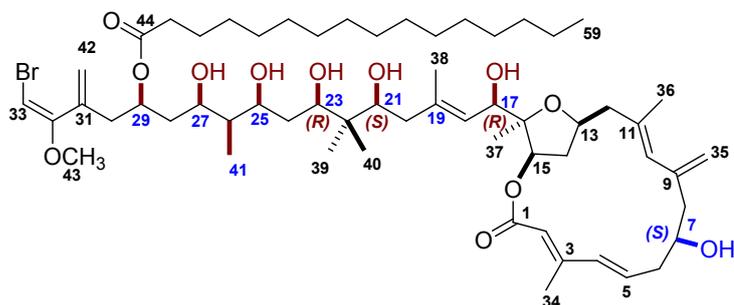


Figure S 11: Epimeric C7 isomers of phormidolide A fragments utilized for DP4 analysis.

### Revised structure of Phormidolide A



### Revised Phormidolide A Structure and Diastereomeric Fragments Utilized

Figure S 12: Re-assigned phormidolide A structure and the eight C24 truncated diastereomeric isomers. Isomer nomenclature is *SRS* for *7S*, *17R* and *21S*. Note that the latter also correspond to *21S/23R*, which are considered a pair and inverted simultaneously).

## Scalar Coupling Constants and $^{13}\text{C}$ Chemical Shifts Analysis

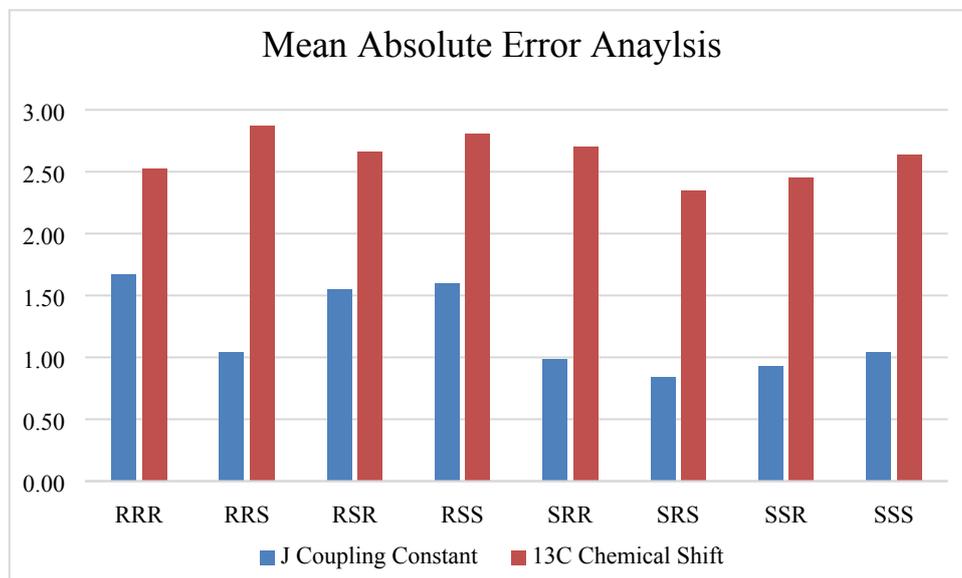


Figure S 13: Mean Absolute Error Analysis of diastereomeric phormidolide isomers (Fig. S12) of experimental vs. theoretical scalar coupling constant (blue) – GIAO-B3LYP<sup>5-8</sup>/6-31G(d)//M06-2X/6-31+G(d,p) – and  $^{13}\text{C}$  chemical shift (red) – GIAO-mPW1PW91<sup>9</sup>/6-311+G(2d,p)//M06-2X/6-31+G(d,p) – values. Chemical shift absolute errors shown includes values from sp<sup>2</sup> carbons which are not well predicted with the DFT functional used.<sup>10,11</sup>

## SVD Analysis of Diastereomeric Phormidolide A Fragments

Due to the moderately flexibility exhibited by these systems, Singular Value decomposition (SVD) analysis<sup>12</sup> of the C24-truncated diastereomeric phormidolide A moieties with the measured RCSAs, included the utilization of Density Functional Theory (DFT) calculated conformer electronic energies (M06-2X<sup>13</sup>/6-31+G(d,p)) to minimize over-fitting of the sparse RCSA data. The SVD fitting protocol was implemented with an in-house developed software program (note that commercially available software packages, such as MagNes,<sup>14</sup> can be utilized as well). SVD analysis is preceded by a global superposition of the coordinates and chemical shielding tensors of all DFT generated low energy conformers of each phormidolide A diastereomers to ensure the smallest RMSD of atomic positions with respect to the principal axis frame of their mass weighted gyration tensors (full details will be published subsequently)<sup>15</sup>. The overlay of seven DFT low energy conformers (Figure S14) generated for the *SRS* truncated moiety indicate the suitability of these systems for utilization of the single-tensor SVD approach. This is then followed by the SVD fitting protocol using five independent variables (RCSA values), with contributions from each conformer weighted with their respective Boltzmann distribution, calculated with DFT derived electronic energies.

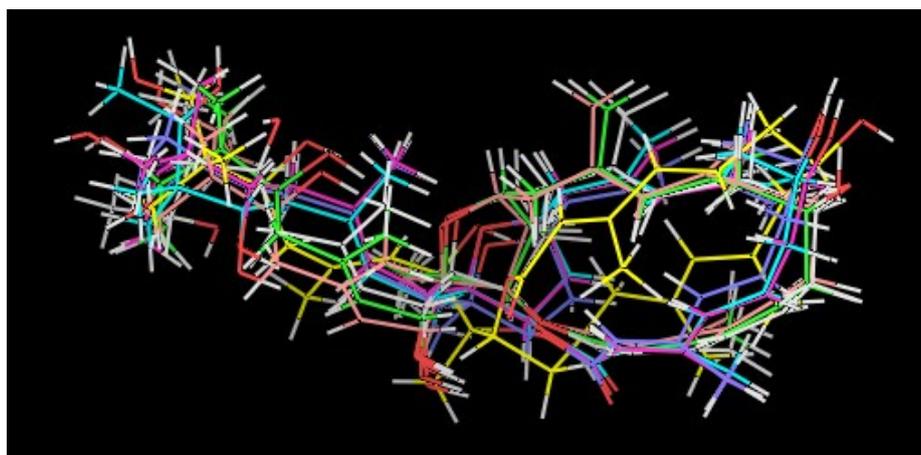


Figure S 14: DFT derived low energy conformers (7 total) of a C24-truncated phormidolide A *SRS* fragment, utilized for the anisotropic NMR study. The overlay indicate suitability of the single-tensor SVD analysis methodology in the structural verification process.

## Conformer Generation and Computation

Conformer generation of macrocyclic systems are not always trivial. To avoid missing out on any low energy conformations for the diastereomeric phormidolide A fragments utilized in this study, two conformer generation tools were used; Macromodel Schrodinger package<sup>16,17</sup> and Forcegen<sup>18</sup>, two softwares that are known to perform better for macrocyclic systems. The conformers were first generated by Prime Macrocycle Sampling tool in Macromodel using OPLS3e forcefield with 20 kcal/mol cutoff, then combined with conformers generated by Forcegen. The combined conformers were first optimized at GAIO-M062X/6-311+G(d,p)-sp//PBE0<sup>19</sup>/Midi<sup>20</sup> level of theory with conformers within 5.0 kcal/mol of the lowest energy conformer (HF energies) selected for the second optimization step (GAIO-M062X/6-311+G(d,p)-sp//M06-2X<sup>13</sup>/6-31+G(d,p) using the int=ultrafine, SMD solvent model<sup>18</sup> and freq=noraman keywords). Chemical shielding tensors were calculated at GIAO-mPW1PW91<sup>9</sup>/6-311+G(2d,p) //M06-2X/6-31+G(d,p). The electronic energies of the *SRS* low energy conformers, optimized geometries and chemical shielding tensors are given below;

Table S 2: DFT electronic energies of conformers of phormidolide A diastereomers calculated with M06-2X<sup>13</sup>/6-31+G(d,p) functional/basis set.

| <b>DFT electronic energies</b> |                   |                   |                   |                   |
|--------------------------------|-------------------|-------------------|-------------------|-------------------|
| <b>Conformers</b>              | <b><i>RRR</i></b> | <b><i>RRS</i></b> | <b><i>RSR</i></b> | <b><i>RSS</i></b> |
| 1                              | -1735.417795      | -1735.418067      | -1735.418076      | -1735.419766      |
| 2                              | -1735.416486      | -1735.417279      | -1735.416766      | -1735.419174      |
| 3                              | -1735.416430      | -1735.417265      | -1735.416577      | -1735.418539      |
| 4                              | -1735.415864      | -1735.416743      | -1735.416084      | -1735.418172      |
| 5                              | -1735.414686      | -1735.416074      | -1735.416047      | -1735.417844      |
| 6                              | -1735.413901      | -1735.416068      | -1735.415897      | -1735.417639      |
| 7                              |                   | -1735.415882      | -1735.415841      | -1735.417534      |
| 8                              |                   | -1735.415865      | -1735.415479      |                   |
| 9                              |                   | -1735.415014      | -1735.414750      |                   |
| 10                             |                   | -1735.414787      | -1735.414721      |                   |
| 11                             |                   | -1735.414660      |                   |                   |
| 12                             |                   | -1735.414657      |                   |                   |
| <b>Conformers</b>              | <b><i>SRR</i></b> | <b><i>SRS</i></b> | <b><i>SSR</i></b> | <b><i>SSS</i></b> |
| 1                              | -1735.421541      | -1735.421094      | -1735.421380      | -1735.421463      |
| 2                              |                   | -1735.419649      | -1735.420359      | -1735.419959      |
| 3                              |                   | -1735.419222      | -1735.419296      | -1735.419931      |
| 4                              |                   | -1735.418336      | -1735.419034      | -1735.418335      |
| 5                              |                   | -1735.417979      | -1735.419016      |                   |
| 6                              |                   | -1735.417442      | -1735.418942      |                   |
| 7                              |                   | -1735.417257      | -1735.418801      |                   |
| 8                              |                   |                   | -1735.418537      |                   |
| 9                              |                   |                   | -1735.417587      |                   |
| 10                             |                   |                   | -1735.417549      |                   |

## DFT Structures of the seven conformations of Phormidolide A (SRS)

| Phormidolide A (SRS) conformer structure coordinates |             |        |        |             |        |        |             |        |        |             |        |        |
|--|-------------|--------|--------|-------------|--------|--------|-------------|--------|--------|-------------|--------|--------|
| DFT numbering  | Conformer 1 |        |        | Conformer 2 |        |        | Conformer 3 |        |        | Conformer 4 |        |        |
| C1   | -2.426      | -2.040 | -1.585 | -0.860      | -0.271 | 1.466  | 2.294       | 2.693  | 0.127  | -2.484      | -2.389 | -1.089 |
| C2   | -3.002      | -0.767 | -2.037 | -1.570      | -1.348 | 0.759  | 3.301       | 2.079  | -0.748 | -3.106      | -1.255 | -1.786 |
| C3   | -4.331      | -0.519 | -2.110 | -2.647      | -2.000 | 1.255  | 4.582       | 1.844  | -0.382 | -4.437      | -1.012 | -1.801 |
| C4   | -4.735      | 0.892  | -2.132 | -3.497      | -2.704 | 0.287  | 5.317       | 0.846  | -1.167 | -4.852      | 0.355  | -2.136 |
| C5   | -5.941      | 1.319  | -1.731 | -4.783      | -3.006 | 0.513  | 6.371       | 0.164  | -0.696 | -6.026      | 0.884  | -1.761 |
| C6   | -6.272      | 2.752  | -1.463 | -5.734      | -3.463 | -0.547 | 6.948       | -1.045 | -1.359 | -6.347      | 2.341  | -1.836 |
| C7   | -6.466      | 3.019  | 0.036  | -6.810      | -2.411 | -0.842 | 6.692       | -2.320 | -0.545 | -6.446      | 2.975  | -0.443 |
| C8   | -5.208      | 2.720  | 0.868  | -6.236      | -1.082 | -1.360 | 5.198       | -2.625 | -0.353 | -5.139      | 2.878  | 0.360  |
| C9   | -4.958      | 1.266  | 1.250  | -5.673      | -0.121 | -0.320 | 4.469       | -1.861 | 0.744  | -4.857      | 1.559  | 1.069  |
| C10  | -3.557      | 0.814  | 1.107  | -4.356      | 0.463  | -0.656 | 3.141       | -1.332 | 0.362  | -3.472      | 1.059  | 0.934  |
| C11  | -2.799      | 0.145  | 1.997  | -3.971      | 1.753  | -0.606 | 1.976       | -1.436 | 1.029  | -2.648      | 0.606  | 1.899  |
| C12  | -1.351      | -0.148 | 1.671  | -2.588      | 2.127  | -1.092 | 0.710       | -0.890 | 0.405  | -1.228      | 0.220  | 1.545  |
| C13  | -0.886      | -1.579 | 1.985  | -1.817      | 3.116  | -0.206 | -0.190      | -0.083 | 1.352  | -0.732      | -1.097 | 2.161  |
| C14  | -1.593      | -2.696 | 1.212  | -1.509      | 2.639  | 1.218  | 0.421       | 1.199  | 1.924  | -1.472      | -2.363 | 1.721  |
| C15  | -0.767      | -2.803 | -0.068 | -0.155      | 1.943  | 1.060  | 0.084       | 2.249  | 0.865  | -0.724      | -2.776 | 0.455  |
| C16  | 0.659       | -2.457 | 0.410  | 0.537       | 2.802  | -0.009 | -1.276      | 1.771  | 0.320  | 0.725       | -2.330 | 0.747  |
| C17  | 1.422       | -1.555 | -0.590 | 1.496       | 2.070  | -0.985 | -1.399      | 1.919  | -1.221 | 1.414       | -1.694 | -0.484 |
| C18  | 2.842       | -1.309 | -0.167 | 2.450       | 1.147  | -0.280 | -2.734      | 1.403  | -1.656 | 2.852       | -1.353 | -0.220 |
| C19  | 3.311       | -0.264 | 0.531  | 3.738       | 1.379  | 0.019  | -3.005      | 0.142  | -2.017 | 3.342       | -0.173 | 0.188  |
| C20  | 4.789       | -0.160 | 0.835  | 4.559       | 0.300  | 0.691  | -4.442      | -0.336 | -2.015 | 4.830       | 0.009  | 0.383  |
| C21  | 5.496       | 0.761  | -0.174 | 5.392       | -0.481 | -0.340 | -4.921      | -0.464 | -0.551 | 5.470       | 0.695  | -0.837 |
| C22  | 6.968       | 1.074  | 0.173  | 6.403       | -1.469 | 0.280  | -6.265      | -1.200 | -0.377 | 6.981       | 1.009  | -0.692 |
| C23  | 7.606       | 1.828  | -1.023 | 7.017       | -2.326 | -0.858 | -6.594      | -1.278 | 1.137  | 7.205       | 1.845  | 0.587  |

|     |        |        |        |
|-----|--------|--------|--------|
| C24 | 6.844  | 3.062  | -1.492 |
| C25 | -5.402 | -1.566 | -1.984 |
| C26 | -5.929 | 0.464  | 1.710  |
| C27 | -3.255 | -0.279 | 3.368  |
| C28 | 1.420  | -3.739 | 0.724  |
| C29 | 2.468  | 0.869  | 1.049  |
| C30 | 7.766  | -0.216 | 0.402  |
| C31 | 7.020  | 1.943  | 1.437  |
| O32 | -1.216 | -1.806 | -1.008 |
| O33 | -6.801 | 4.401  | 0.124  |
| O34 | 0.494  | -1.710 | 1.625  |
| O35 | 1.481  | -2.178 | -1.870 |
| O36 | 5.465  | 0.173  | -1.470 |
| O37 | 8.930  | 2.197  | -0.623 |
| H38 | -2.303 | 0.064  | -2.074 |
| H39 | -6.246 | -1.323 | -2.636 |
| H40 | -5.777 | -1.584 | -0.952 |
| H41 | -5.031 | -2.557 | -2.230 |
| H42 | -3.952 | 1.622  | -2.338 |
| H43 | -6.715 | 0.593  | -1.487 |
| H44 | -5.473 | 3.408  | -1.827 |
| H45 | -7.203 | 3.034  | -1.969 |
| H46 | -7.306 | 2.413  | 0.402  |
| H47 | -7.001 | 4.615  | 1.045  |
| H48 | -4.337 | 3.116  | 0.331  |
| H49 | -5.277 | 3.299  | 1.799  |
| H50 | -5.724 | -0.572 | 1.966  |
| H51 | -6.952 | 0.808  | 1.835  |

|        |        |        |
|--------|--------|--------|
| 7.606  | -1.534 | -2.019 |
| -3.128 | -1.899 | 2.676  |
| -6.334 | 0.189  | 0.804  |
| -4.847 | 2.901  | -0.181 |
| 1.282  | 3.952  | 0.666  |
| 4.482  | 2.654  | -0.277 |
| 5.711  | -2.417 | 1.269  |
| 7.504  | -0.682 | 1.004  |
| -0.389 | 0.619  | 0.561  |
| -7.647 | -3.006 | -1.829 |
| -0.529 | 3.342  | -0.810 |
| 0.784  | 1.305  | -1.943 |
| 4.530  | -1.217 | -1.202 |
| 8.029  | -3.144 | -0.262 |
| -1.340 | -1.426 | -0.300 |
| -3.471 | -2.877 | 3.026  |
| -3.985 | -1.214 | 2.726  |
| -2.352 | -1.532 | 3.342  |
| -3.083 | -2.847 | -0.712 |
| -5.211 | -2.833 | 1.500  |
| -5.198 | -3.677 | -1.479 |
| -6.249 | -4.378 | -0.233 |
| -7.392 | -2.229 | 0.073  |
| -8.377 | -2.404 | -2.026 |
| -5.468 | -1.309 | -2.110 |
| -7.039 | -0.558 | -1.896 |
| -5.906 | 0.866  | 1.539  |
| -7.311 | -0.230 | 1.032  |

|        |        |        |
|--------|--------|--------|
| -6.517 | 0.044  | 1.892  |
| 5.228  | 2.386  | 0.863  |
| 4.979  | -1.705 | 1.975  |
| 1.797  | -2.145 | 2.345  |
| -2.403 | 2.477  | 1.065  |
| -1.982 | -0.930 | -2.272 |
| -6.181 | -2.638 | -0.909 |
| -7.362 | -0.435 | -1.128 |
| 1.064  | 2.202  | -0.188 |
| 7.319  | -3.362 | -1.285 |
| -1.344 | 0.364  | 0.624  |
| -1.280 | 3.286  | -1.592 |
| -3.955 | -1.124 | 0.261  |
| -7.912 | -1.825 | 1.248  |
| 2.901  | 1.586  | -1.629 |
| 6.276  | 2.631  | 0.668  |
| 5.211  | 1.618  | 1.648  |
| 4.715  | 3.269  | 1.235  |
| 4.874  | 0.550  | -2.119 |
| 6.795  | 0.430  | 0.272  |
| 6.514  | -1.183 | -2.356 |
| 8.034  | -0.941 | -1.472 |
| 7.179  | -2.222 | 0.436  |
| 7.246  | -4.188 | -0.788 |
| 4.690  | -2.468 | -1.313 |
| 5.101  | -3.696 | -0.131 |
| 4.442  | -1.146 | 2.736  |
| 5.945  | -2.117 | 2.256  |

|        |        |        |
|--------|--------|--------|
| 8.607  | 2.423  | 0.733  |
| -5.487 | -1.977 | -1.325 |
| -5.789 | 0.914  | 1.786  |
| -2.996 | 0.528  | 3.362  |
| 1.519  | -3.504 | 1.307  |
| 2.509  | 1.048  | 0.475  |
| 7.417  | 1.791  | -1.939 |
| 7.792  | -0.290 | -0.592 |
| -1.241 | -2.031 | -0.666 |
| -6.781 | 4.339  | -0.681 |
| 0.626  | -1.317 | 1.759  |
| 1.401  | -2.606 | -1.579 |
| 5.320  | -0.130 | -1.990 |
| 6.239  | 2.899  | 0.592  |
| -2.418 | -0.469 | -2.085 |
| -6.376 | -1.909 | -1.959 |
| -5.790 | -1.712 | -0.303 |
| -5.125 | -3.001 | -1.321 |
| -4.093 | 1.002  | -2.577 |
| -6.774 | 0.250  | -1.286 |
| -5.576 | 2.878  | -2.402 |
| -7.309 | 2.500  | -2.338 |
| -7.260 | 2.489  | 0.113  |
| -6.902 | 4.784  | 0.168  |
| -4.305 | 3.123  | -0.309 |
| -5.156 | 3.668  | 1.124  |
| -5.566 | -0.032 | 2.272  |
| -6.799 | 1.300  | 1.902  |

|     |        |        |        |        |        |        |        |        |        |        |        |        |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| H52 | -3.075 | 1.127  | 0.179  | -3.637 | -0.253 | -1.058 | 3.112  | -0.856 | -0.620 | -3.062 | 1.134  | -0.074 |
| H53 | -3.451 | -1.359 | 3.405  | -4.568 | 3.264  | 0.816  | 1.681  | -1.430 | 3.169  | -3.186 | -0.507 | 3.671  |
| H54 | -4.169 | 0.234  | 3.673  | -5.903 | 2.624  | -0.152 | 2.645  | -2.791 | 2.582  | -3.884 | 1.116  | 3.604  |
| H55 | -2.469 | -0.073 | 4.104  | -4.721 | 3.743  | -0.872 | 0.885  | -2.753 | 2.322  | -2.156 | 0.890  | 3.966  |
| H56 | -1.152 | 0.068  | 0.616  | -1.982 | 1.223  | -1.215 | 0.956  | -0.272 | -0.466 | -1.112 | 0.173  | 0.457  |
| H57 | -0.713 | 0.517  | 2.271  | -2.680 | 2.606  | -2.078 | 0.100  | -1.733 | 0.050  | -0.549 | 1.002  | 1.916  |
| H58 | -0.951 | -1.751 | 3.065  | -2.338 | 4.079  | -0.191 | -0.554 | -0.735 | 2.153  | -0.729 | -1.007 | 3.253  |
| H59 | -2.648 | -2.491 | 1.009  | -2.270 | 1.962  | 1.619  | 1.497  | 1.126  | 2.107  | -2.540 | -2.208 | 1.540  |
| H60 | -1.526 | -3.637 | 1.766  | -1.417 | 3.490  | 1.897  | -0.070 | 1.463  | 2.865  | -1.362 | -3.145 | 2.478  |
| H61 | -0.815 | -3.784 | -0.544 | 0.427  | 1.889  | 1.982  | 0.032  | 3.267  | 1.257  | -0.789 | -3.842 | 0.231  |
| H62 | 2.315  | -3.505 | 1.306  | 1.606  | 4.671  | -0.092 | -3.349 | 1.955  | 0.895  | 2.445  | -3.141 | 1.760  |
| H63 | 0.796  | -4.417 | 1.315  | 0.632  | 4.474  | 1.375  | -2.204 | 2.475  | 2.142  | 0.940  | -4.022 | 2.079  |
| H64 | 1.716  | -4.248 | -0.199 | 2.159  | 3.585  | 1.207  | -2.502 | 3.512  | 0.725  | 1.764  | -4.216 | 0.513  |
| H65 | 0.872  | -0.610 | -0.656 | 2.048  | 2.865  | -1.505 | -0.591 | 1.334  | -1.669 | 0.847  | -0.792 | -0.739 |
| H66 | 0.597  | -2.136 | -2.262 | 0.027  | 1.846  | -2.213 | -0.351 | 3.542  | -1.500 | 0.496  | -2.651 | -1.916 |
| H67 | 3.538  | -2.097 | -0.460 | 2.009  | 0.194  | 0.010  | -3.565 | 2.095  | -1.504 | 3.544  | -2.184 | -0.367 |
| H68 | 1.471  | 0.900  | 0.606  | 3.947  | 3.320  | -0.956 | -0.953 | -0.569 | -2.255 | 1.494  | 0.978  | 0.081  |
| H69 | 2.962  | 1.832  | 0.872  | 5.464  | 2.436  | -0.712 | -2.173 | -1.387 | -3.251 | 2.986  | 1.945  | 0.067  |
| H70 | 2.344  | 0.766  | 2.134  | 4.667  | 3.200  | 0.656  | -2.082 | -1.728 | -1.527 | 2.433  | 1.191  | 1.560  |
| H71 | 5.254  | -1.149 | 0.787  | 3.901  | -0.404 | 1.210  | -4.517 | -1.298 | -2.531 | 5.314  | -0.962 | 0.537  |
| H72 | 4.925  | 0.236  | 1.849  | 5.227  | 0.756  | 1.430  | -5.091 | 0.380  | -2.531 | 4.997  | 0.627  | 1.272  |
| H73 | 4.954  | 1.720  | -0.202 | 5.966  | 0.243  | -0.940 | -5.053 | 0.565  | -0.181 | 4.956  | 1.650  | -1.011 |
| H74 | 4.565  | -0.142 | -1.637 | 3.825  | -0.627 | -1.505 | -3.146 | -0.585 | 0.306  | 4.395  | -0.409 | -2.041 |
| H75 | 7.654  | -0.899 | -0.447 | 4.848  | -2.904 | 0.802  | -5.310 | -3.155 | -0.494 | 6.930  | 2.772  | -1.974 |
| H76 | 8.827  | 0.019  | 0.519  | 6.410  | -3.191 | 1.595  | -7.081 | -3.189 | -0.624 | 8.501  | 1.944  | -1.952 |
| H77 | 7.435  | -0.734 | 1.307  | 5.364  | -1.881 | 2.158  | -6.109 | -2.661 | -2.001 | 7.144  | 1.238  | -2.841 |
| H78 | 6.351  | 2.809  | 1.367  | 7.937  | 0.097  | 0.368  | -7.389 | 0.624  | -0.848 | 7.598  | -0.823 | 0.345  |
| H79 | 6.731  | 1.367  | 2.321  | 7.113  | -0.200 | 1.905  | -7.202 | -0.492 | -2.209 | 7.538  | -0.954 | -1.422 |

|     |        |        |        |        |        |        |        |        |        |        |        |        |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| H80 | 8.037  | 2.311  | 1.597  | 8.307  | -1.358 | 1.310  | -8.341 | -0.870 | -0.911 | 8.866  | -0.083 | -0.643 |
| H81 | 7.671  | 1.118  | -1.857 | 6.218  | -2.972 | -1.243 | -5.878 | -1.979 | 1.586  | 7.019  | 1.188  | 1.450  |
| H82 | 9.402  | 2.518  | -1.402 | 8.316  | -3.793 | -0.917 | -8.073 | -2.036 | 2.177  | 6.424  | 3.482  | 1.339  |
| H83 | 7.410  | 3.559  | -2.287 | 8.077  | -2.224 | -2.728 | -6.867 | -0.104 | 2.920  | 8.697  | 2.928  | 1.701  |
| H84 | 6.708  | 3.780  | -0.677 | 8.372  | -0.831 | -1.676 | -7.148 | 0.809  | 1.429  | 8.813  | 3.155  | -0.053 |
| H85 | 5.867  | 2.793  | -1.902 | 6.830  | -0.986 | -2.561 | -5.488 | 0.411  | 1.947  | 9.371  | 1.641  | 0.698  |
| O86 | -2.921 | -3.147 | -1.612 | -0.748 | -0.102 | 2.664  | 2.461  | 3.456  | 1.056  | -2.966 | -3.471 | -0.824 |

| Phormidolide A ( <i>SRS</i> ) conformer structure coordinates |             |        |        |             |        |        |             |        |        |  |  |  |
|---|-------------|--------|--------|-------------|--------|--------|-------------|--------|--------|--|--|--|
| DFT numbering   | Conformer 5 |        |        | Conformer 6 |        |        | Conformer 7 |        |        |  |  |  |
| C1  | 2.275       | 2.696  | -0.070 | 2.366       | 2.618  | -0.336 | -2.405      | -2.311 | -1.225 |  |  |  |
| C2  | 3.233       | 2.033  | -0.965 | 3.288       | 1.868  | -1.198 | -3.073      | -1.170 | -1.865 |  |  |  |
| C3  | 4.541       | 1.847  | -0.674 | 4.620       | 1.764  | -0.980 | -4.414      | -0.991 | -1.888 |  |  |  |
| C4  | 5.242       | 0.804  | -1.434 | 5.309       | 0.648  | -1.639 | -4.890      | 0.373  | -2.150 |  |  |  |
| C5  | 6.347       | 0.185  | -0.993 | 6.463       | 0.128  | -1.196 | -6.093      | 0.822  | -1.766 |  |  |  |
| C6  | 6.902       | -1.065 | -1.594 | 7.022       | -1.180 | -1.655 | -6.481      | 2.265  | -1.758 |  |  |  |
| C7  | 6.720       | -2.281 | -0.666 | 6.921       | -2.263 | -0.563 | -6.623      | 2.807  | -0.329 |  |  |  |
| C8  | 5.248       | -2.577 | -0.342 | 5.475       | -2.542 | -0.125 | -5.321      | 2.713  | 0.483  |  |  |  |
| C9  | 4.591       | -1.734 | 0.745  | 4.855       | -1.580 | 0.880  | -4.993      | 1.367  | 1.115  |  |  |  |
| C10   | 3.223       | -1.266 | 0.433  | 3.453       | -1.202 | 0.598  | -3.582      | 0.942  | 0.980  |  |  |  |
| C11   | 2.120       | -1.333 | 1.203  | 2.401       | -1.197 | 1.439  | -2.753      | 0.475  | 1.933  |  |  |  |
| C12   | 0.793       | -0.870 | 0.644  | 1.027       | -0.848 | 0.913  | -1.310      | 0.183  | 1.588  |  |  |  |
| C13   | -0.047      | 0.001  | 1.589  | 0.216       | 0.122  | 1.788  | -0.761      | -1.146 | 2.131  |  |  |  |
| C14   | 0.573       | 1.342  | 1.989  | 0.820       | 1.516  | 1.977  | -1.431      | -2.415 | 1.597  |  |  |  |
| C15   | 0.134       | 2.278  | 0.863  | 0.290       | 2.285  | 0.769  | -0.646      | -2.705 | 0.319  |  |  |  |



|     |        |        |        |        |        |        |        |        |        |  |  |  |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--|--|--|
| H44 | 6.405  | -1.279 | -2.549 | 6.481  | -1.532 | -2.543 | -5.731 | 2.870  | -2.280 |  |  |  |
| H45 | 7.977  | -0.959 | -1.785 | 8.081  | -1.079 | -1.917 | -7.445 | 2.409  | -2.260 |  |  |  |
| H46 | 7.276  | -2.110 | 0.262  | 7.517  | -1.957 | 0.303  | -7.422 | 2.255  | 0.185  |  |  |  |
| H47 | 6.884  | -3.624 | -2.083 | 7.047  | -3.784 | -1.792 | -7.158 | 4.555  | 0.386  |  |  |  |
| H48 | 4.661  | -2.492 | -1.267 | 4.841  | -2.587 | -1.021 | -4.491 | 3.031  | -0.161 |  |  |  |
| H49 | 5.190  | -3.628 | -0.035 | 5.459  | -3.547 | 0.315  | -5.376 | 3.454  | 1.292  |  |  |  |
| H50 | 4.709  | -0.854 | 2.666  | 5.057  | -0.441 | 2.652  | -5.644 | -0.327 | 2.204  |  |  |  |
| H51 | 6.193  | -1.831 | 2.143  | 6.544  | -1.433 | 2.165  | -6.934 | 0.965  | 1.890  |  |  |  |
| H52 | 3.100  | -0.877 | -0.579 | 3.255  | -0.957 | -0.447 | -3.160 | 1.095  | -0.015 |  |  |  |
| H53 | 2.002  | -1.146 | 3.352  | 2.409  | -0.724 | 3.547  | -3.266 | -0.767 | 3.626  |  |  |  |
| H54 | 2.952  | -2.533 | 2.804  | 3.373  | -2.146 | 3.128  | -4.044 | 0.821  | 3.640  |  |  |  |
| H55 | 1.176  | -2.554 | 2.690  | 1.595  | -2.231 | 3.136  | -2.313 | 0.660  | 4.023  |  |  |  |
| H56 | 0.950  | -0.327 | -0.295 | 1.106  | -0.435 | -0.099 | -1.170 | 0.211  | 0.502  |  |  |  |
| H57 | 0.179  | -1.753 | 0.416  | 0.429  | -1.769 | 0.849  | -0.679 | 0.971  | 2.024  |  |  |  |
| H58 | -0.325 | -0.583 | 2.473  | 0.012  | -0.350 | 2.755  | -0.781 | -1.125 | 3.226  |  |  |  |
| H59 | 1.661  | 1.306  | 2.098  | 1.913  | 1.521  | 2.024  | -2.503 | -2.302 | 1.408  |  |  |  |
| H60 | 0.144  | 1.687  | 2.933  | 0.435  | 1.971  | 2.894  | -1.291 | -3.239 | 2.303  |  |  |  |
| H61 | 0.082  | 3.327  | 1.160  | 0.226  | 3.364  | 0.924  | -0.652 | -3.756 | 0.026  |  |  |  |
| H62 | -3.281 | 1.938  | 1.163  | -3.102 | 1.915  | 1.272  | 2.528  | -2.996 | 1.632  |  |  |  |
| H63 | -2.066 | 2.621  | 2.254  | -1.863 | 2.748  | 2.229  | 1.070  | -3.973 | 1.873  |  |  |  |
| H64 | -2.486 | 3.478  | 0.751  | -2.355 | 3.408  | 0.650  | 1.912  | -4.014 | 0.306  |  |  |  |
| H65 | -0.686 | 1.073  | -1.504 | -0.652 | 0.710  | -1.344 | 0.825  | -0.559 | -0.709 |  |  |  |
| H66 | -0.481 | 3.291  | -1.588 | -0.372 | 2.889  | -1.737 | 0.596  | -2.348 | -2.022 |  |  |  |
| H67 | -3.656 | 1.816  | -1.234 | -3.551 | 1.660  | -1.269 | 3.594  | -1.815 | -0.403 |  |  |  |
| H68 | -1.051 | -0.885 | -1.864 | -1.170 | -1.268 | -1.305 | 1.356  | 1.179  | 0.262  |  |  |  |
| H69 | -2.315 | -1.820 | -2.689 | -2.465 | -2.331 | -1.899 | 2.788  | 2.225  | 0.387  |  |  |  |
| H70 | -2.115 | -1.970 | -0.947 | -2.295 | -2.026 | -0.172 | 2.243  | 1.295  | 1.783  |  |  |  |
| H71 | -4.620 | -1.677 | -1.850 | -4.760 | -1.453 | -2.249 | 5.273  | -0.575 | 0.614  |  |  |  |

|     |        |        |        |        |        |        |        |        |        |  |  |  |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--|--|--|
| H72 | -5.214 | -0.028 | -2.028 | -5.157 | 0.185  | -1.715 | 4.872  | 0.915  | 1.489  |  |  |  |
| H73 | -5.060 | 0.436  | 0.309  | -4.908 | -0.724 | 0.700  | 4.728  | 2.099  | -0.759 |  |  |  |
| H74 | -3.127 | -0.639 | 0.799  | -4.899 | -3.157 | -0.715 | 4.440  | 0.072  | -1.916 |  |  |  |
| H75 | -6.502 | -0.064 | 2.150  | -6.996 | -1.079 | 2.032  | 6.442  | 2.429  | 1.705  |  |  |  |
| H76 | -7.519 | -1.519 | 2.156  | -8.351 | -1.945 | 1.277  | 7.664  | 3.334  | 0.811  |  |  |  |
| H77 | -5.779 | -1.640 | 2.478  | -6.785 | -2.747 | 1.468  | 5.946  | 3.575  | 0.444  |  |  |  |
| H78 | -5.995 | -3.091 | -0.920 | -7.087 | -1.861 | -2.229 | 7.364  | 1.624  | -2.460 |  |  |  |
| H79 | -5.322 | -3.273 | 0.715  | -7.044 | -3.225 | -1.091 | 6.657  | 3.164  | -1.964 |  |  |  |
| H80 | -7.075 | -3.354 | 0.452  | -8.478 | -2.216 | -1.194 | 8.316  | 2.761  | -1.479 |  |  |  |
| H81 | -8.360 | -1.257 | 0.051  | -7.162 | 0.401  | -1.430 | 7.317  | 0.258  | 1.127  |  |  |  |
| H82 | -8.158 | -0.922 | -2.240 | -6.858 | 1.928  | 0.354  | 9.605  | 0.587  | 0.749  |  |  |  |
| H83 | -8.574 | 0.996  | -0.882 | -9.078 | 1.405  | -0.335 | 8.651  | -1.268 | -0.283 |  |  |  |
| H84 | -6.819 | 1.227  | -0.880 | -8.987 | 0.263  | 1.018  | 8.370  | -0.248 | -1.708 |  |  |  |
| H85 | -7.709 | 1.092  | 0.654  | -9.438 | -0.301 | -0.608 | 7.014  | -1.097 | -0.951 |  |  |  |
| O86 | 2.489  | 3.540  | 0.776  | 2.603  | 3.569  | 0.380  | -2.835 | -3.429 | -1.031 |  |  |  |

## Chemical Shielding Tensors of the seven conformations of Phormidolide A (SRS)

### Conformer 1

1 C Isotropic = 13.8484 Anisotropy = 87.3354

XX= -36.8464 YX= 37.5388 ZX= -67.6043

XY= 14.0602 YY= 43.6056 ZY= 13.2255

XZ= -55.8182 YZ= 30.4180 ZZ= 34.7858

Eigenvalues: -81.2521 50.7252 72.0720

2 C Isotropic = 65.0329 Anisotropy = 103.1237

XX= 76.2431 YX= -29.1016 ZX= 3.0615

XY= -24.5591 YY= -12.5524 ZY= 24.6426

XZ= 2.6309 YZ= 12.5863 ZZ= 131.4081

Eigenvalues: -22.3043 83.6210 133.7821

3 C Isotropic = 22.2749 Anisotropy = 207.3356

XX= -8.6274 YX= -3.5255 ZX= 4.5211

XY= -12.5305 YY= -82.2465 ZY= 21.2993

XZ= 2.6269 YZ= 30.4335 ZZ= 157.6986

Eigenvalues: -85.9083 -7.7656 160.4987

4 C Isotropic = 45.7590 Anisotropy = 121.6916

XX= 44.3507 YX= -50.6733 ZX= 29.5852

XY= -52.1468 YY= -22.9275 ZY= 15.7170

XZ= 30.1123 YZ= 10.8731 ZZ= 115.8539

Eigenvalues: -54.7296 65.1199 126.8868

5 C Isotropic = 41.5297 Anisotropy = 185.9261

XX= 29.4577 YX= -33.1773 ZX= 43.6752

XY= -39.3707 YY= -56.4702 ZY= -3.0930

XZ= 42.1206 YZ= 8.7349 ZZ= 151.6016

Eigenvalues: -71.1796 30.2883 165.4804

6 C Isotropic = 141.2439 Anisotropy = 22.1198

XX= 121.6903 YX= -5.0093 ZX= 1.4473

XY= 1.2822 YY= 148.5626 ZY= 3.2788

XZ= -2.3285 YZ= 5.2431 ZZ= 153.4787

Eigenvalues: 121.5610 146.1803 155.9904

7 C Isotropic = 110.2477 Anisotropy = 48.0581

XX= 99.1890 YX= -12.6950 ZX= 5.7848

XY= -13.2844 YY= 138.2282 ZY= 3.6102

XZ= 5.0735 YZ= 4.9200 ZZ= 93.3261

Eigenvalues: 87.7236 100.7331 142.2865

8 C Isotropic = 138.9169 Anisotropy = 40.6938

XX= 137.7436 YX= -17.6226 ZX= 19.4457

XY= -11.4999 YY= 145.5400 ZY= -8.3567

XZ= 13.8628 YZ= -8.9423 ZZ= 133.4669

Eigenvalues: 118.3034 132.4011 166.0460

9 C Isotropic = 33.9852 Anisotropy = 178.6965

XX= -11.4020 YX= 65.3914 ZX= 11.5594

XY= 64.1247 YY= -20.9739 ZY= 45.0647

XZ= 15.4971 YZ= 46.7763 ZZ= 134.3314

Eigenvalues: -84.0277 32.8671 153.1162

10 C Isotropic = 47.4881 Anisotropy = 108.9556

XX= 12.9543 YX= -3.3992 ZX= 61.0514

XY= -6.4858 YY= 112.2012 ZY= 26.1781

XZ= 62.8973 YZ= 24.9458 ZZ= 17.3087  
 Eigenvalues: -49.7167 72.0558 120.1252  
 11 C Isotropic = 41.8996 Anisotropy = 175.2916  
 XX= -17.4333 YX= 25.4616 ZX= 61.5731  
 XY= 36.3914 YY= 128.5265 ZY= 46.7479  
 XZ= 53.4212 YZ= 44.6104 ZZ= 14.6055  
 Eigenvalues: -61.1557 28.0938 158.7606  
 12 C Isotropic = 135.5929 Anisotropy = 40.1232  
 XX= 153.5182 YX= -10.0167 ZX= -15.6800  
 XY= -14.1480 YY= 132.0211 ZY= 3.0636  
 XZ= -11.6851 YZ= -7.4340 ZZ= 121.2394  
 Eigenvalues: 113.7690 130.6681 162.3417  
 13 C Isotropic = 105.5532 Anisotropy = 79.8400  
 XX= 152.5560 YX= -1.9960 ZX= -21.1829  
 XY= -5.6965 YY= 83.3713 ZY= 18.6137  
 XZ= -20.3823 YZ= 5.9669 ZZ= 80.7321  
 Eigenvalues: 67.4660 90.4137 158.7798  
 14 C Isotropic = 150.1174 Anisotropy = 30.1211  
 XX= 152.0949 YX= -5.9399 ZX= -3.0081  
 XY= 7.0136 YY= 137.1529 ZY= 16.8465  
 XZ= -11.0279 YZ= 12.5868 ZZ= 161.1045  
 Eigenvalues: 129.5868 150.5674 170.1981  
 15 C Isotropic = 103.1525 Anisotropy = 31.5955  
 XX= 111.4755 YX= -14.0154 ZX= 9.8229  
 XY= -8.7022 YY= 88.8699 ZY= -19.0552  
 XZ= -3.6794 YZ= -13.5329 ZZ= 109.1119  
 Eigenvalues: 77.6011 107.6401 124.2162  
 16 C Isotropic = 95.5718 Anisotropy = 63.3804  
 XX= 87.5600 YX= 3.1267 ZX= -14.0792  
 XY= 0.2707 YY= 77.0002 ZY= 25.2919  
 XZ= -6.3850 YZ= 32.8686 ZZ= 122.1552  
 Eigenvalues: 61.3261 87.5639 137.8254  
 17 C Isotropic = 112.2290 Anisotropy = 42.1583  
 XX= 97.2410 YX= 3.5201 ZX= -10.2932  
 XY= 8.2496 YY= 102.0365 ZY= 7.4834  
 XZ= -2.3605 YZ= 11.5473 ZZ= 137.4094  
 Eigenvalues: 90.8242 105.5282 140.3345  
 18 C Isotropic = 52.5359 Anisotropy = 115.6623  
 XX= -13.2165 YX= 58.7838 ZX= 3.5621  
 XY= 55.8469 YY= 51.2833 ZY= -26.4254  
 XZ= 9.4316 YZ= -25.3929 ZZ= 119.5410  
 Eigenvalues: -48.8402 76.8039 129.6441  
 19 C Isotropic = 40.8598 Anisotropy = 175.4326  
 XX= -49.3952 YX= 47.8638 ZX= -12.6723  
 XY= 39.2124 YY= 53.1696 ZY= -57.0013  
 XZ= -9.9288 YZ= -59.3528 ZZ= 118.8050  
 Eigenvalues: -65.9441 30.7087 157.8149  
 20 C Isotropic = 142.6661 Anisotropy = 23.3574  
 XX= 158.2330 YX= -2.0877 ZX= -1.9628  
 XY= 1.8890 YY= 134.9795 ZY= -0.3815  
 XZ= 2.5569 YZ= -6.7608 ZZ= 134.7857  
 Eigenvalues: 131.3094 138.4512 158.2377  
 21 C Isotropic = 112.6749 Anisotropy = 36.6441  
 XX= 108.5274 YX= 7.4639 ZX= 13.6926  
 XY= 1.0861 YY= 104.5115 ZY= 17.9405

XZ= 2.6365 YZ= 14.9826 ZZ= 124.9859  
 Eigenvalues: 95.3588 105.5617 137.1043  
 22 C Isotropic = 143.7073 Anisotropy = 18.5281  
 XX= 147.7460 YX= 13.3318 ZX= 2.0853  
 XY= 8.1253 YY= 142.1748 ZY= 0.8873  
 XZ= -2.4552 YZ= -1.9346 ZZ= 141.2012  
 Eigenvalues: 133.8637 141.1989 156.0594  
 23 C Isotropic = 113.2499 Anisotropy = 44.3996  
 XX= 136.1192 YX= 17.2948 ZX= 7.9541  
 XY= 10.1292 YY= 107.0206 ZY= -6.4986  
 XZ= 12.6752 YZ= -4.5323 ZZ= 96.6100  
 Eigenvalues: 89.1188 107.7813 142.8497  
 24 C Isotropic = 167.2542 Anisotropy = 29.4064  
 XX= 172.0287 YX= -4.7563 ZX= 6.5108  
 XY= -13.3184 YY= 174.6579 ZY= -10.3842  
 XZ= 6.9735 YZ= -9.1262 ZZ= 155.0761  
 Eigenvalues: 150.5958 164.3083 186.8585  
 25 C Isotropic = 171.9070 Anisotropy = 15.8088  
 XX= 167.8085 YX= 11.3963 ZX= 4.8984  
 XY= 14.3229 YY= 169.5148 ZY= 0.1451  
 XZ= 1.3930 YZ= -0.9776 ZZ= 178.3977  
 Eigenvalues: 155.4814 177.7934 182.4462  
 26 C Isotropic = 69.1145 Anisotropy = 144.3488  
 XX= 31.7373 YX= 59.7109 ZX= 9.9301  
 XY= 59.1926 YY= 16.8936 ZY= 27.9903  
 XZ= 2.0891 YZ= 22.3899 ZZ= 158.7127  
 Eigenvalues: -36.7564 78.7529 165.3470  
 27 C Isotropic = 167.8359 Anisotropy = 27.1103  
 XX= 159.5709 YX= 1.8646 ZX= -5.5302  
 XY= 6.3763 YY= 160.6052 ZY= 9.4506  
 XZ= -6.8113 YZ= 3.0477 ZZ= 183.3316  
 Eigenvalues: 153.3703 164.2280 185.9094  
 28 C Isotropic = 165.8759 Anisotropy = 31.4048  
 XX= 166.0079 YX= -12.0872 ZX= 3.9556  
 XY= -16.3913 YY= 176.9624 ZY= 5.3540  
 XZ= 7.1726 YZ= -1.3146 ZZ= 154.6574  
 Eigenvalues: 149.6257 161.1896 186.8124  
 29 C Isotropic = 166.6470 Anisotropy = 20.0333  
 XX= 169.2160 YX= -7.1675 ZX= -2.8488  
 XY= -13.0050 YY= 169.1701 ZY= 3.3484  
 XZ= -6.0003 YZ= -1.9687 ZZ= 161.5547  
 Eigenvalues: 157.2388 162.6996 180.0025  
 30 C Isotropic = 168.9439 Anisotropy = 30.8793  
 XX= 156.7930 YX= -18.2166 ZX= -5.2362  
 XY= -9.4319 YY= 183.6684 ZY= -0.3540  
 XZ= -5.8824 YZ= -2.8785 ZZ= 166.3704  
 Eigenvalues: 149.0423 168.2593 189.5302  
 31 C Isotropic = 170.4567 Anisotropy = 29.8463  
 XX= 158.4762 YX= -2.3222 ZX= 2.1268  
 XY= -4.9700 YY= 178.8423 ZY= 10.3229  
 XZ= 2.2355 YZ= 16.9507 ZZ= 174.0515  
 Eigenvalues: 155.9839 165.0319 190.3542  
 32 O Isotropic = 103.0754 Anisotropy = 131.7974  
 XX= 190.5262 YX= -29.3252 ZX= 5.5030  
 XY= 41.0131 YY= -31.1237 ZY= 111.2291

XZ= -13.7454 YZ= 13.0068 ZZ= 149.8238  
 Eigenvalues: -50.5877 168.8736 190.9404  
 33 O Isotropic = 255.7761 Anisotropy = 91.5282  
 XX= 224.3758 YX= -34.6643 ZX= 12.4983  
 XY= -35.5540 YY= 249.9079 ZY= 27.7551  
 XZ= -5.5676 YZ= 46.0075 ZZ= 293.0447  
 Eigenvalues: 193.3747 257.1587 316.7950  
 34 O Isotropic = 220.6980 Anisotropy = 80.4676  
 XX= 258.8669 YX= 14.8156 ZX= 0.0439  
 XY= 23.0804 YY= 183.8840 ZY= 63.5080  
 XZ= -1.4438 YZ= 59.8149 ZZ= 219.3432  
 Eigenvalues: 135.4778 252.2732 274.3431  
 35 O Isotropic = 277.9052 Anisotropy = 73.0141  
 XX= 299.9068 YX= 13.8225 ZX= 36.4297  
 XY= 10.0215 YY= 247.0250 ZY= 22.0167  
 XZ= 17.0514 YZ= 16.1853 ZZ= 286.7838  
 Eigenvalues: 239.3100 267.8243 326.5812  
 36 O Isotropic = 278.8983 Anisotropy = 26.5232  
 XX= 294.2569 YX= 7.2933 ZX= -18.6711  
 XY= 1.7693 YY= 286.6743 ZY= 22.5081  
 XZ= 3.6284 YZ= -1.5655 ZZ= 255.7637  
 Eigenvalues: 250.8729 289.2415 296.5804  
 37 O Isotropic = 266.7118 Anisotropy = 61.9731  
 XX= 283.3388 YX= 4.2106 ZX= -7.3146  
 XY= 15.9494 YY= 247.2535 ZY= -29.5047  
 XZ= -23.8437 YZ= -38.3575 ZZ= 269.5432  
 Eigenvalues: 222.6669 269.4413 308.0272  
 38 H Isotropic = 25.8497 Anisotropy = 8.8373  
 XX= 28.7076 YX= -3.3403 ZX= 1.4320  
 XY= -5.2258 YY= 23.5258 ZY= -0.5617  
 XZ= 1.9878 YZ= -1.4932 ZZ= 25.3157  
 Eigenvalues: 21.1102 24.6977 31.7412  
 39 H Isotropic = 30.1375 Anisotropy = 8.5827  
 XX= 32.1820 YX= -0.8795 ZX= 4.4971  
 XY= 0.6579 YY= 29.0888 ZY= 0.8185  
 XZ= 5.3772 YZ= 1.0316 ZZ= 29.1418  
 Eigenvalues: 25.3210 29.2322 35.8593  
 40 H Isotropic = 30.1574 Anisotropy = 6.0528  
 XX= 29.4545 YX= 0.4439 ZX= -1.6552  
 XY= 0.8312 YY= 28.1519 ZY= 0.3128  
 XZ= -3.3444 YZ= -0.0758 ZZ= 32.8658  
 Eigenvalues: 27.5210 28.7586 34.1926  
 41 H Isotropic = 27.9232 Anisotropy = 7.9260  
 XX= 29.6393 YX= -1.0354 ZX= 1.7872  
 XY= -3.1646 YY= 31.6894 ZY= 2.2619  
 XZ= 1.3537 YZ= 2.9564 ZZ= 22.4409  
 Eigenvalues: 21.2394 29.3230 33.2072  
 42 H Isotropic = 25.2256 Anisotropy = 6.4112  
 XX= 25.8261 YX= -4.0645 ZX= -0.1350  
 XY= -4.8101 YY= 24.0870 ZY= 0.6723  
 XZ= -0.1404 YZ= -0.1154 ZZ= 25.7638  
 Eigenvalues: 20.4318 25.7454 29.4997  
 43 H Isotropic = 25.3680 Anisotropy = 7.3858  
 XX= 24.5633 YX= -3.1071 ZX= 1.4531  
 XY= -4.8096 YY= 26.8214 ZY= 3.2728

XZ= 1.1645 YZ= 2.4747 ZZ= 24.7194  
 Eigenvalues: 19.8984 25.9138 30.2919  
 44 H Isotropic = 29.6840 Anisotropy = 4.0038  
 XX= 28.8269 YX= -1.1549 ZX= -1.5589  
 XY= 0.7724 YY= 30.5528 ZY= -1.8333  
 XZ= -2.2225 YZ= -1.8267 ZZ= 29.6724  
 Eigenvalues: 26.8127 29.8862 32.3532  
 45 H Isotropic = 28.7461 Anisotropy = 7.7137  
 XX= 30.1799 YX= -2.1542 ZX= 3.0011  
 XY= -2.5623 YY= 27.1786 ZY= 0.2273  
 XZ= 4.3640 YZ= -0.8528 ZZ= 28.8798  
 Eigenvalues: 24.8897 27.4600 33.8886  
 46 H Isotropic = 27.5784 Anisotropy = 3.8056  
 XX= 28.1358 YX= -0.7141 ZX= -1.6693  
 XY= 0.5810 YY= 29.7052 ZY= -1.7113  
 XZ= -1.5005 YZ= -0.9350 ZZ= 24.8942  
 Eigenvalues: 23.9734 28.6463 30.1154  
 47 H Isotropic = 31.5230 Anisotropy = 16.8102  
 XX= 25.2014 YX= -3.8265 ZX= -3.5798  
 XY= -4.5207 YY= 31.8553 ZY= 6.5656  
 XZ= -4.1430 YZ= 4.7330 ZZ= 37.5122  
 Eigenvalues: 23.0873 28.7518 42.7298  
 48 H Isotropic = 29.9124 Anisotropy = 3.8815  
 XX= 32.2318 YX= -0.8661 ZX= 0.3254  
 XY= -0.7497 YY= 29.5033 ZY= -1.5244  
 XZ= 0.3757 YZ= 0.6170 ZZ= 28.0021  
 Eigenvalues: 27.8719 29.3652 32.5001  
 49 H Isotropic = 29.5951 Anisotropy = 5.3586  
 XX= 26.5029 YX= -0.4199 ZX= 1.8153  
 XY= -2.6581 YY= 31.0705 ZY= 1.3231  
 XZ= 0.6600 YZ= 2.7159 ZZ= 31.2119  
 Eigenvalues: 25.4460 30.1718 33.1675  
 50 H Isotropic = 26.7567 Anisotropy = 5.3598  
 XX= 29.2307 YX= 3.5765 ZX= -1.0085  
 XY= 1.4542 YY= 24.4932 ZY= -0.2990  
 XZ= 0.7438 YZ= -0.1977 ZZ= 26.5461  
 Eigenvalues: 23.3971 26.5431 30.3299  
 51 H Isotropic = 26.6051 Anisotropy = 6.2808  
 XX= 26.2552 YX= 0.4814 ZX= -0.8109  
 XY= 3.8880 YY= 26.3119 ZY= -2.7878  
 XZ= -2.7151 YZ= -1.7759 ZZ= 27.2482  
 Eigenvalues: 24.0119 25.0112 30.7923  
 52 H Isotropic = 26.0650 Anisotropy = 8.8379  
 XX= 27.6364 YX= -4.2260 ZX= 4.1199  
 XY= -4.0977 YY= 25.9353 ZY= 0.0359  
 XZ= 3.2267 YZ= 1.2185 ZZ= 24.6233  
 Eigenvalues: 20.3889 25.8491 31.9569  
 53 H Isotropic = 30.4132 Anisotropy = 5.9899  
 XX= 28.9692 YX= 1.0757 ZX= -2.6695  
 XY= 0.6545 YY= 33.1564 ZY= -1.8498  
 XZ= -2.1522 YZ= -1.7182 ZZ= 29.1140  
 Eigenvalues: 26.5638 30.2693 34.4064  
 54 H Isotropic = 29.4709 Anisotropy = 6.6438  
 XX= 31.7311 YX= -3.8232 ZX= -0.3297  
 XY= -3.5190 YY= 26.1719 ZY= -0.1436

XZ= -2.0199 YZ= 0.2520 ZZ= 30.5097  
 Eigenvalues: 24.3097 30.2028 33.9001  
 55 H Isotropic = 30.4569 Anisotropy = 8.1074  
 XX= 30.7977 YX= -0.6221 ZX= 0.9836  
 XY= 0.2899 YY= 25.8110 ZY= 2.7253  
 XZ= 2.8867 YZ= 1.2069 ZZ= 34.7620  
 Eigenvalues: 25.3368 30.1721 35.8618  
 56 H Isotropic = 29.0095 Anisotropy = 4.5666  
 XX= 29.9634 YX= -2.4228 ZX= -1.6793  
 XY= -2.6047 YY= 28.5135 ZY= 0.3116  
 XZ= 0.0240 YZ= 0.2623 ZZ= 28.5518  
 Eigenvalues: 26.5830 28.3917 32.0539  
 57 H Isotropic = 29.0900 Anisotropy = 4.8928  
 XX= 31.5840 YX= -0.0623 ZX= 0.6094  
 XY= 2.0966 YY= 29.6081 ZY= 2.6507  
 XZ= 0.0233 YZ= 2.3691 ZZ= 26.0779  
 Eigenvalues: 24.7693 30.1489 32.3519  
 58 H Isotropic = 27.3298 Anisotropy = 6.9726  
 XX= 27.4605 YX= -1.8272 ZX= -3.3854  
 XY= -1.9946 YY= 24.1326 ZY= -0.3557  
 XZ= -1.7457 YZ= 0.0610 ZZ= 30.3963  
 Eigenvalues: 23.0382 26.9730 31.9782  
 59 H Isotropic = 30.0017 Anisotropy = 6.0792  
 XX= 34.0476 YX= 0.0148 ZX= 0.4550  
 XY= -0.3671 YY= 27.4452 ZY= 1.5217  
 XZ= -0.1774 YZ= 0.7919 ZZ= 28.5122  
 Eigenvalues: 26.6980 29.2525 34.0545  
 60 H Isotropic = 29.5979 Anisotropy = 9.3923  
 XX= 27.0407 YX= 1.0828 ZX= -1.3788  
 XY= 1.6540 YY= 32.7606 ZY= -3.7116  
 XZ= -2.0932 YZ= -4.4296 ZZ= 28.9923  
 Eigenvalues: 25.7564 27.1778 35.8594  
 61 H Isotropic = 26.5907 Anisotropy = 3.2549  
 XX= 26.7624 YX= -1.7039 ZX= 1.7760  
 XY= -0.5591 YY= 28.1144 ZY= 1.9826  
 XZ= 2.7660 YZ= 0.7575 ZZ= 24.8953  
 Eigenvalues: 22.7862 28.2253 28.7606  
 62 H Isotropic = 30.6206 Anisotropy = 7.8414  
 XX= 34.2482 YX= 0.5418 ZX= 3.2780  
 XY= -0.6684 YY= 29.9800 ZY= -2.0382  
 XZ= 3.6057 YZ= -2.0510 ZZ= 27.6336  
 Eigenvalues: 25.4028 30.6108 35.8482  
 63 H Isotropic = 31.1183 Anisotropy = 7.7929  
 XX= 31.0611 YX= -0.3395 ZX= -1.0022  
 XY= 0.0937 YY= 34.3541 ZY= -4.1377  
 XZ= -1.0183 YZ= -3.9104 ZZ= 27.9395  
 Eigenvalues: 25.8234 31.2179 36.3135  
 64 H Isotropic = 30.1503 Anisotropy = 8.9852  
 XX= 28.2257 YX= -2.6849 ZX= -2.3464  
 XY= -3.2050 YY= 33.0568 ZY= 3.4801  
 XZ= -2.0317 YZ= 2.0059 ZZ= 29.1684  
 Eigenvalues: 26.3582 27.9524 36.1405  
 65 H Isotropic = 26.7875 Anisotropy = 3.1883  
 XX= 28.1266 YX= 1.0010 ZX= -0.2957  
 XY= 0.8291 YY= 27.1345 ZY= 1.3870

XZ= 0.4899 YZ= 1.6812 ZZ= 25.1016  
 Eigenvalues: 24.2450 27.2045 28.9131  
 66 H Isotropic = 30.3538 Anisotropy = 17.0020  
 XX= 39.2181 YX= -1.1186 ZX= 4.5806  
 XY= -0.2892 YY= 19.9014 ZY= 2.2622  
 XZ= 5.2268 YZ= 1.5814 ZZ= 31.9421  
 Eigenvalues: 19.4851 29.8879 41.6885  
 67 H Isotropic = 26.0901 Anisotropy = 9.9730  
 XX= 28.6870 YX= 5.2890 ZX= 0.8695  
 XY= 4.5665 YY= 26.7109 ZY= 0.3251  
 XZ= -0.1174 YZ= -0.0715 ZZ= 22.8724  
 Eigenvalues: 22.5977 22.9338 32.7388  
 68 H Isotropic = 29.5714 Anisotropy = 9.2747  
 XX= 35.4276 YX= 2.0475 ZX= 1.5477  
 XY= -0.3923 YY= 28.6246 ZY= 0.6090  
 XZ= 1.3286 YZ= 1.9106 ZZ= 24.6620  
 Eigenvalues: 24.1748 28.7849 35.7546  
 69 H Isotropic = 30.1491 Anisotropy = 7.3775  
 XX= 32.3482 YX= 1.2244 ZX= -1.7767  
 XY= 2.1910 YY= 33.7717 ZY= 0.2167  
 XZ= -1.7061 YZ= -0.9611 ZZ= 24.3273  
 Eigenvalues: 23.9655 31.4143 35.0674  
 70 H Isotropic = 30.1690 Anisotropy = 7.0269  
 XX= 30.3295 YX= 1.0680 ZX= -2.5568  
 XY= 1.4303 YY= 26.6451 ZY= 1.6093  
 XZ= -2.0745 YZ= 1.7366 ZZ= 33.5325  
 Eigenvalues: 25.5594 30.0941 34.8536  
 71 H Isotropic = 29.7123 Anisotropy = 6.4435  
 XX= 33.8258 YX= 0.2490 ZX= 0.3763  
 XY= 1.0243 YY= 30.9979 ZY= -1.8209  
 XZ= 1.8206 YZ= -2.7554 ZZ= 24.3131  
 Eigenvalues: 23.4571 31.6718 34.0080  
 72 H Isotropic = 29.5092 Anisotropy = 5.4549  
 XX= 32.2791 YX= 3.2489 ZX= -0.3631  
 XY= 2.0611 YY= 24.9488 ZY= 0.6247  
 XZ= 0.0358 YZ= 1.0566 ZZ= 31.2997  
 Eigenvalues: 23.9893 31.3925 33.1458  
 73 H Isotropic = 28.4396 Anisotropy = 3.6596  
 XX= 30.2061 YX= 0.3480 ZX= -1.4480  
 XY= 0.6874 YY= 29.4088 ZY= -0.1342  
 XZ= -1.8494 YZ= 0.4599 ZZ= 25.7041  
 Eigenvalues: 25.1413 29.2983 30.8794  
 74 H Isotropic = 30.3238 Anisotropy = 21.0734  
 XX= 39.7175 YX= 8.7737 ZX= 3.6180  
 XY= 9.6708 YY= 22.4984 ZY= 0.5756  
 XZ= 1.7019 YZ= 3.1425 ZZ= 28.7556  
 Eigenvalues: 18.4495 28.1493 44.3728  
 75 H Isotropic = 30.5375 Anisotropy = 8.5225  
 XX= 29.6787 YX= -2.3184 ZX= -0.7161  
 XY= -1.8225 YY= 33.2702 ZY= 4.5392  
 XZ= 0.3642 YZ= 3.6724 ZZ= 28.6635  
 Eigenvalues: 26.0165 29.3768 36.2192  
 76 H Isotropic = 30.1598 Anisotropy = 8.6431  
 XX= 35.6331 YX= -0.8349 ZX= 1.0334  
 XY= -1.1744 YY= 29.3871 ZY= -1.6454

XZ= 0.7084 YZ= -2.0547 ZZ= 25.4591  
 Eigenvalues: 24.7068 29.8506 35.9218  
 77 H Isotropic = 31.3562 Anisotropy = 7.7847  
 XX= 30.7399 YX= -0.9162 ZX= 0.3584  
 XY= -0.3197 YY= 32.0353 ZY= -5.0160  
 XZ= -0.2257 YZ= -4.6330 ZZ= 31.2933  
 Eigenvalues: 26.7904 30.7322 36.5460  
 78 H Isotropic = 31.2083 Anisotropy = 8.3827  
 XX= 29.3449 YX= -2.3201 ZX= -0.9933  
 XY= -3.0621 YY= 34.6595 ZY= 1.7372  
 XZ= -1.4348 YZ= 3.0895 ZZ= 29.6204  
 Eigenvalues: 28.1508 28.6772 36.7967  
 79 H Isotropic = 31.3530 Anisotropy = 7.2425  
 XX= 29.1412 YX= 2.0185 ZX= -0.6660  
 XY= 1.7603 YY= 28.9366 ZY= -0.4906  
 XZ= -0.8468 YZ= -0.8945 ZZ= 35.9810  
 Eigenvalues: 27.1467 30.7309 36.1813  
 80 H Isotropic = 30.1514 Anisotropy = 9.1359  
 XX= 32.3923 YX= 3.7940 ZX= 1.5704  
 XY= 4.2170 YY= 27.6013 ZY= 2.4465  
 XZ= 2.2992 YZ= 2.8033 ZZ= 30.4606  
 Eigenvalues: 24.9459 29.2662 36.2419  
 81 H Isotropic = 27.6021 Anisotropy = 3.5875  
 XX= 28.3908 YX= 2.9787 ZX= 0.0377  
 XY= 1.4519 YY= 26.4506 ZY= 1.8700  
 XZ= -1.1999 YZ= 1.6076 ZZ= 27.9649  
 Eigenvalues: 24.1661 28.6464 29.9937  
 82 H Isotropic = 31.8225 Anisotropy = 18.9931  
 XX= 36.1248 YX= 5.2842 ZX= -7.1657  
 XY= 4.8519 YY= 25.4365 ZY= -5.4512  
 XZ= -6.4319 YZ= -4.2678 ZZ= 33.9062  
 Eigenvalues: 22.8281 28.1548 44.4846  
 83 H Isotropic = 31.0699 Anisotropy = 9.9815  
 XX= 29.3111 YX= 0.8645 ZX= -1.8585  
 XY= 1.9703 YY= 31.2166 ZY= -5.1966  
 XZ= -2.1468 YZ= -4.8282 ZZ= 32.6821  
 Eigenvalues: 26.8535 28.6320 37.7243  
 84 H Isotropic = 30.6638 Anisotropy = 6.1016  
 XX= 27.2707 YX= -1.0791 ZX= -1.4794  
 XY= -0.8025 YY= 34.4907 ZY= 1.1761  
 XZ= -1.0839 YZ= -0.0532 ZZ= 30.2299  
 Eigenvalues: 26.7308 30.5291 34.7315  
 85 H Isotropic = 30.2451 Anisotropy = 7.6360  
 XX= 33.5218 YX= 1.3570 ZX= 3.6695  
 XY= 0.9337 YY= 28.9788 ZY= -3.3536  
 XZ= 3.3941 YZ= -3.3568 ZZ= 28.2347  
 Eigenvalues: 23.9853 31.4143 35.3358  
 86 O Isotropic = -90.0805 Anisotropy = 613.7607  
 XX= -168.7574 YX= -114.2952 ZX= -219.9429  
 XY= -112.7239 YY= -290.5425 ZY= 80.6359  
 XZ= -204.1711 YZ= 117.8727 ZZ= 189.0584  
 Eigenvalues: -360.1150 -229.2198 319.0933

## Conformer 2

1 C Isotropic = 13.3230 Anisotropy = 90.9132

XX= 42.4367 YX= -61.1340 ZX= 12.5300

XY= -58.6616 YY= -40.3173 ZY= 13.0225

XZ= 20.2638 YZ= 43.2695 ZZ= 37.8497

Eigenvalues: -80.6756 46.7128 73.9318

2 C Isotropic = 63.0788 Anisotropy = 106.6574

XX= 95.8182 YX= -30.7461 ZX= -3.4221

XY= -25.7288 YY= 100.0488 ZY= -41.0691

XZ= -3.5673 YZ= -50.6983 ZZ= -6.6305

Eigenvalues: -25.1231 80.1758 134.1838

3 C Isotropic = 25.3029 Anisotropy = 203.3106

XX= 40.1903 YX= -76.3117 ZX= 1.2557

XY= -82.3902 YY= 89.6922 ZY= -66.6784

XZ= 6.9136 YZ= -55.5586 ZZ= -53.9740

Eigenvalues: -82.4242 -2.5104 160.8432

4 C Isotropic = 45.5862 Anisotropy = 121.8024

XX= 66.8906 YX= -10.1801 ZX= 14.8270

XY= -8.7291 YY= 110.8973 ZY= -44.2451

XZ= 17.7875 YZ= -47.6081 ZZ= -41.0294

Eigenvalues: -55.2653 65.2360 126.7877

5 C Isotropic = 43.5321 Anisotropy = 182.4191

XX= 42.4017 YX= -29.8824 ZX= 3.7517

XY= -35.8354 YY= 139.9159 ZY= -64.0273

XZ= 5.7027 YZ= -52.7843 ZZ= -51.7213

Eigenvalues: -68.2959 33.7473 165.1449

6 C Isotropic = 141.3663 Anisotropy = 22.2834

XX= 139.3965 YX= -7.8667 ZX= 15.9605

XY= -12.4743 YY= 144.2574 ZY= 4.9821

XZ= 11.6549 YZ= 1.5401 ZZ= 140.4451

Eigenvalues: 121.8657 146.0113 156.2220

7 C Isotropic = 109.6906 Anisotropy = 47.5322

XX= 107.6021 YX= 16.2919 ZX= 20.2003

XY= 15.5774 YY= 105.2246 ZY= 8.8505

XZ= 20.6251 YZ= 10.1763 ZZ= 116.2452

Eigenvalues: 87.3945 100.2987 141.3787

8 C Isotropic = 139.0013 Anisotropy = 40.3597

XX= 129.0171 YX= 19.6112 ZX= 9.3658

XY= 13.9810 YY= 157.0872 ZY= 5.7167

XZ= 6.9496 YZ= -0.6617 ZZ= 130.8995

Eigenvalues: 117.9132 133.1829 165.9077

9 C Isotropic = 34.0586 Anisotropy = 177.9747

XX= -3.8021 YX= -95.2681 ZX= 4.3413

XY= -91.3796 YY= 52.7111 ZY= -65.9430

XZ= 2.5138 YZ= -62.7389 ZZ= 53.2668

Eigenvalues: -83.3841 32.8514 152.7084

10 C Isotropic = 46.3609 Anisotropy = 111.8957

XX= -6.4583 YX= 37.0005 ZX= 58.8163

XY= 39.3270 YY= 53.2371 ZY= -17.8218

XZ= 61.9315 YZ= -15.0908 ZZ= 92.3039

Eigenvalues: -51.5405 69.6651 120.9580

11 C Isotropic = 43.5594 Anisotropy = 172.4625

XX= -28.3646 YX= 15.8119 ZX= 72.7970

XY= 8.0074 YY= 28.9618 ZY= -15.7010

XZ= 67.6669 YZ= -25.8441 ZZ= 130.0812  
 Eigenvalues: -58.9560 31.0999 158.5345  
 12 C Isotropic = 136.8356 Anisotropy = 40.8508  
 XX= 160.1650 YX= 6.6971 ZX= -10.1057  
 XY= 16.2481 YY= 124.2473 ZY= 9.0743  
 XZ= -3.5842 YZ= 5.9515 ZZ= 126.0945  
 Eigenvalues: 113.8537 132.5837 164.0694  
 13 C Isotropic = 106.1010 Anisotropy = 80.3740  
 XX= 147.5185 YX= 7.3735 ZX= -27.3547  
 XY= 14.7003 YY= 70.9952 ZY= -8.0148  
 XZ= -20.2635 YZ= -13.4703 ZZ= 99.7893  
 Eigenvalues: 67.2850 91.3343 159.6836  
 14 C Isotropic = 149.6840 Anisotropy = 32.9916  
 XX= 165.4381 YX= -8.2205 ZX= 3.1960  
 XY= -15.8337 YY= 141.8773 ZY= -3.8411  
 XZ= 0.3205 YZ= -17.3069 ZZ= 141.7365  
 Eigenvalues: 129.5825 147.7910 171.6783  
 15 C Isotropic = 105.7926 Anisotropy = 30.4964  
 XX= 107.9713 YX= 11.8245 ZX= -9.6600  
 XY= -3.7111 YY= 125.1639 ZY= 5.0899  
 XZ= -11.9997 YZ= 2.4916 ZZ= 84.2427  
 Eigenvalues: 79.4934 111.7610 126.1236  
 16 C Isotropic = 95.8347 Anisotropy = 59.9094  
 XX= 115.5224 YX= -24.5723 ZX= 16.9076  
 XY= -13.7498 YY= 80.6478 ZY= -21.9196  
 XZ= 16.2233 YZ= -14.3466 ZZ= 91.3340  
 Eigenvalues: 66.2086 85.5213 135.7743  
 17 C Isotropic = 111.7961 Anisotropy = 38.1805  
 XX= 106.2413 YX= 6.4629 ZX= 1.0645  
 XY= 10.9825 YY= 109.1381 ZY= 17.0446  
 XZ= 8.4791 YZ= 21.4302 ZZ= 120.0090  
 Eigenvalues: 93.0942 105.0444 137.2498  
 18 C Isotropic = 50.7925 Anisotropy = 118.7469  
 XX= 74.2431 YX= -14.2815 ZX= -7.8747  
 XY= -11.8743 YY= -24.2217 ZY= 65.4890  
 XZ= -4.1721 YZ= 59.3134 ZZ= 102.3560  
 Eigenvalues: -50.5869 73.0072 129.9571  
 19 C Isotropic = 39.9497 Anisotropy = 175.4013  
 XX= 44.6565 YX= -6.0126 ZX= -37.7254  
 XY= -10.7161 YY= -38.2851 ZY= 77.1202  
 XZ= -34.9442 YZ= 74.3831 ZZ= 113.4775  
 Eigenvalues: -69.9749 32.9400 156.8838  
 20 C Isotropic = 142.7703 Anisotropy = 21.8394  
 XX= 138.8926 YX= -11.2466 ZX= 3.8172  
 XY= -7.3958 YY= 150.2403 ZY= -3.5420  
 XZ= -1.9884 YZ= -8.6548 ZZ= 139.1781  
 Eigenvalues: 132.6984 138.2826 157.3300  
 21 C Isotropic = 112.8429 Anisotropy = 37.3983  
 XX= 120.1967 YX= 11.7254 ZX= 20.7824  
 XY= 0.5724 YY= 107.3627 ZY= 2.4662  
 XZ= 17.9809 YZ= 8.7637 ZZ= 110.9693  
 Eigenvalues: 95.6244 105.1292 137.7751  
 22 C Isotropic = 143.6586 Anisotropy = 18.7995  
 XX= 151.0984 YX= -4.8065 ZX= 1.4783  
 XY= -12.9448 YY= 140.4685 ZY= 2.3937

XZ= -0.1623 YZ= 4.0336 ZZ= 139.4088  
 Eigenvalues: 133.7145 141.0696 156.1916  
 23 C Isotropic = 113.7961 Anisotropy = 43.9367  
 XX= 123.3132 YX= -20.8078 ZX= 0.8806  
 XY= -24.2170 YY= 109.5796 ZY= -8.8603  
 XZ= 7.8363 YZ= -13.7693 ZZ= 108.4956  
 Eigenvalues: 90.2863 108.0149 143.0873  
 24 C Isotropic = 167.2561 Anisotropy = 29.5043  
 XX= 163.4381 YX= 2.6658 ZX= -11.1191  
 XY= -4.2860 YY= 164.8448 ZY= -14.5875  
 XZ= -5.7451 YZ= -16.3019 ZZ= 173.4854  
 Eigenvalues: 150.3698 164.4729 186.9257  
 25 C Isotropic = 172.4329 Anisotropy = 14.7838  
 XX= 161.7121 YX= -7.1074 ZX= -3.9870  
 XY= -10.6905 YY= 174.5851 ZY= -1.4548  
 XZ= -4.3558 YZ= -4.7629 ZZ= 181.0016  
 Eigenvalues: 156.1078 178.9022 182.2888  
 26 C Isotropic = 68.9005 Anisotropy = 143.7000  
 XX= 34.0438 YX= -82.5004 ZX= -11.7520  
 XY= -85.7682 YY= 90.5229 ZY= -43.0677  
 XZ= -5.2649 YZ= -48.8908 ZZ= 82.1348  
 Eigenvalues: -36.5380 78.5390 164.7005  
 27 C Isotropic = 168.0404 Anisotropy = 27.7523  
 XX= 171.2215 YX= -16.9359 ZX= 2.9123  
 XY= -15.2820 YY= 167.8659 ZY= 0.4059  
 XZ= 1.9008 YZ= -7.4649 ZZ= 165.0336  
 Eigenvalues: 153.2568 164.3224 186.5419  
 28 C Isotropic = 161.1150 Anisotropy = 34.9385  
 XX= 157.9941 YX= 12.2318 ZX= 10.9652  
 XY= 17.6481 YY= 167.4114 ZY= 7.4093  
 XZ= 9.7191 YZ= 8.5734 ZZ= 157.9394  
 Eigenvalues: 145.3629 153.5747 184.4073  
 29 C Isotropic = 168.0251 Anisotropy = 21.1509  
 XX= 161.5166 YX= 12.0428 ZX= -2.7654  
 XY= 3.3091 YY= 176.8490 ZY= -3.5059  
 XZ= -6.1514 YZ= -5.3972 ZZ= 165.7097  
 Eigenvalues: 157.4698 164.4798 182.1257  
 30 C Isotropic = 168.6990 Anisotropy = 31.2673  
 XX= 164.9206 YX= 12.3760 ZX= -9.4948  
 XY= 18.0164 YY= 171.2262 ZY= -4.2673  
 XZ= -15.6312 YZ= -1.9385 ZZ= 169.9503  
 Eigenvalues: 149.1325 167.4207 189.5439  
 31 C Isotropic = 170.4883 Anisotropy = 30.0085  
 XX= 178.9751 YX= 15.4711 ZX= 1.8825  
 XY= 15.2933 YY= 166.6875 ZY= 0.8032  
 XZ= 8.6926 YZ= 2.1266 ZZ= 165.8022  
 Eigenvalues: 155.9287 165.0422 190.4939  
 32 O Isotropic = 97.5475 Anisotropy = 143.1422  
 XX= 173.1812 YX= -57.7452 ZX= -50.9308  
 XY= -25.5273 YY= 81.8196 ZY= -43.8334  
 XZ= -58.8535 YZ= -169.9596 ZZ= 37.6417  
 Eigenvalues: -69.0024 168.6692 192.9756  
 33 O Isotropic = 254.8783 Anisotropy = 90.9709  
 XX= 281.6233 YX= -1.8715 ZX= 47.2118  
 XY= -26.8734 YY= 265.0701 ZY= -21.7995

XZ= 46.5660 YZ= -14.6589 ZZ= 217.9414  
 Eigenvalues: 191.8343 257.2750 315.5256  
 34 O Isotropic = 220.9020 Anisotropy = 82.7653  
 XX= 254.5031 YX= -4.0197 ZX= -6.2776  
 XY= -12.6910 YY= 162.4617 ZY= -50.2109  
 XZ= -16.1744 YZ= -62.4835 ZZ= 245.7412  
 Eigenvalues: 132.7485 253.8786 276.0789  
 35 O Isotropic = 277.5767 Anisotropy = 47.9720  
 XX= 303.1194 YX= -7.5957 ZX= 27.0973  
 XY= -12.7108 YY= 280.0121 ZY= 13.6422  
 XZ= -0.5124 YZ= -13.6787 ZZ= 249.5987  
 Eigenvalues: 246.3139 276.8582 309.5581  
 36 O Isotropic = 279.1130 Anisotropy = 24.1536  
 XX= 292.8188 YX= -1.2955 ZX= 3.2703  
 XY= -4.4775 YY= 291.2042 ZY= 8.2514  
 XZ= -7.5431 YZ= -22.6462 ZZ= 253.3161  
 Eigenvalues: 251.8265 290.2972 295.2154  
 37 O Isotropic = 266.3219 Anisotropy = 63.0361  
 XX= 244.2996 YX= -33.0336 ZX= -9.3619  
 XY= -32.7711 YY= 273.7190 ZY= 3.6214  
 XZ= -26.7814 YZ= 17.5723 ZZ= 280.9471  
 Eigenvalues: 221.3574 269.2623 308.3460  
 38 H Isotropic = 25.7677 Anisotropy = 8.8466  
 XX= 28.4950 YX= 2.7842 ZX= -1.0754  
 XY= 3.8051 YY= 28.1679 ZY= -0.9581  
 XZ= 0.6951 YZ= -0.4517 ZZ= 20.6404  
 Eigenvalues: 20.5729 25.0649 31.6655  
 39 H Isotropic = 30.2702 Anisotropy = 8.6797  
 XX= 27.6457 YX= 2.4970 ZX= 0.9188  
 XY= 2.9257 YY= 32.4222 ZY= -3.7412  
 XZ= -0.7253 YZ= -3.9804 ZZ= 30.7429  
 Eigenvalues: 25.6377 29.1163 36.0567  
 40 H Isotropic = 30.3131 Anisotropy = 6.5884  
 XX= 32.6790 YX= -2.4324 ZX= -0.8208  
 XY= -3.8903 YY= 29.5030 ZY= 0.8611  
 XZ= -0.4776 YZ= -0.3962 ZZ= 28.7572  
 Eigenvalues: 27.5356 28.6983 34.7053  
 41 H Isotropic = 27.9142 Anisotropy = 8.4486  
 XX= 29.6547 YX= 5.3328 ZX= 1.3873  
 XY= 4.7871 YY= 24.6064 ZY= -1.1354  
 XZ= 3.2258 YZ= 0.1858 ZZ= 29.4813  
 Eigenvalues: 21.1522 29.0438 33.5465  
 42 H Isotropic = 25.2507 Anisotropy = 6.9387  
 XX= 28.8031 YX= 1.4261 ZX= 1.0303  
 XY= 1.9024 YY= 26.3948 ZY= 0.2989  
 XZ= 2.0369 YZ= 0.0159 ZZ= 20.5543  
 Eigenvalues: 20.2750 25.6007 29.8765  
 43 H Isotropic = 25.4593 Anisotropy = 7.6058  
 XX= 27.7740 YX= 1.9361 ZX= 3.1788  
 XY= 2.3559 YY= 25.1911 ZY= -1.2549  
 XZ= 4.9734 YZ= -1.0986 ZZ= 23.4129  
 Eigenvalues: 20.0725 25.7756 30.5298  
 44 H Isotropic = 29.6896 Anisotropy = 3.8391  
 XX= 30.4675 YX= -0.1825 ZX= 0.2066  
 XY= -1.0064 YY= 29.3396 ZY= 3.2403

XZ= -1.1599 YZ= 2.0105 ZZ= 29.2617  
 Eigenvalues: 26.6733 30.1465 32.2490  
 45 H Isotropic = 28.7858 Anisotropy = 7.5631  
 XX= 27.8028 YX= 1.7204 ZX= 0.4915  
 XY= 3.5074 YY= 32.3020 ZY= -1.9443  
 XZ= 0.7313 YZ= -2.0179 ZZ= 26.2527  
 Eigenvalues: 24.8728 27.6568 33.8279  
 46 H Isotropic = 27.5847 Anisotropy = 3.6187  
 XX= 28.3027 YX= 1.3771 ZX= 0.1220  
 XY= 1.0249 YY= 25.8624 ZY= 2.4341  
 XZ= -1.3276 YZ= 2.3800 ZZ= 28.5891  
 Eigenvalues: 24.0376 28.7194 29.9972  
 47 H Isotropic = 31.5534 Anisotropy = 16.8369  
 XX= 37.7612 YX= -5.2142 ZX= 6.1721  
 XY= -4.5726 YY= 29.8314 ZY= 0.2478  
 XZ= 7.6778 YZ= -0.9202 ZZ= 27.0676  
 Eigenvalues: 23.0545 28.8276 42.7780  
 48 H Isotropic = 29.9655 Anisotropy = 3.4902  
 XX= 30.5998 YX= 2.5545 ZX= -0.2148  
 XY= 1.3653 YY= 29.5903 ZY= -0.9278  
 XZ= -1.2135 YZ= 0.5943 ZZ= 29.7064  
 Eigenvalues: 28.0123 29.5920 32.2923  
 49 H Isotropic = 29.5657 Anisotropy = 5.6838  
 XX= 29.4330 YX= -0.1168 ZX= 2.9528  
 XY= -1.5206 YY= 30.3879 ZY= -1.4423  
 XZ= 4.7641 YZ= 0.2899 ZZ= 28.8761  
 Eigenvalues: 25.2824 30.0598 33.3549  
 50 H Isotropic = 26.7392 Anisotropy = 5.2714  
 XX= 26.4482 YX= -1.5392 ZX= -3.4244  
 XY= 0.2636 YY= 25.9181 ZY= -2.2477  
 XZ= -2.4702 YZ= -0.1617 ZZ= 27.8513  
 Eigenvalues: 23.4722 26.4919 30.2535  
 51 H Isotropic = 26.5222 Anisotropy = 6.2447  
 XX= 25.8140 YX= -0.6836 ZX= -0.9932  
 XY= -3.1895 YY= 26.4657 ZY= 2.8738  
 XZ= -3.4870 YZ= 1.0620 ZZ= 27.2868  
 Eigenvalues: 24.0087 24.8725 30.6853  
 52 H Isotropic = 25.9928 Anisotropy = 8.7545  
 XX= 26.5478 YX= 4.7555 ZX= 2.3413  
 XY= 3.5732 YY= 28.5452 ZY= -1.9078  
 XZ= 2.1138 YZ= -1.6669 ZZ= 22.8852  
 Eigenvalues: 20.2125 25.9367 31.8291  
 53 H Isotropic = 30.4719 Anisotropy = 5.6786  
 XX= 30.5406 YX= -1.0118 ZX= 0.0719  
 XY= -0.4526 YY= 29.1190 ZY= 3.2576  
 XZ= 0.1675 YZ= 3.8534 ZZ= 31.7560  
 Eigenvalues: 26.5332 30.6248 34.2576  
 54 H Isotropic = 29.3871 Anisotropy = 6.6527  
 XX= 33.6563 YX= 1.4936 ZX= -0.5481  
 XY= -0.1566 YY= 30.3436 ZY= -0.3044  
 XZ= -0.4364 YZ= -0.8045 ZZ= 24.1614  
 Eigenvalues: 24.0924 30.2466 33.8222  
 55 H Isotropic = 30.4134 Anisotropy = 8.5708  
 XX= 30.3124 YX= -3.1007 ZX= 0.8364  
 XY= -0.7796 YY= 33.1593 ZY= -3.8223

XZ= -0.1121 YZ= -4.7327 ZZ= 27.7685  
 Eigenvalues: 25.3251 29.7878 36.1273  
 56 H Isotropic = 28.8541 Anisotropy = 5.8082  
 XX= 32.3744 YX= -0.5683 ZX= 1.5614  
 XY= 1.8101 YY= 29.0830 ZY= 0.1200  
 XZ= 0.9761 YZ= 0.9731 ZZ= 25.1050  
 Eigenvalues: 24.8446 28.9915 32.7262  
 57 H Isotropic = 29.1667 Anisotropy = 5.0555  
 XX= 29.4467 YX= 1.2647 ZX= 2.1323  
 XY= 1.0878 YY= 26.4431 ZY= -1.0019  
 XZ= 0.7315 YZ= -2.5263 ZZ= 31.6104  
 Eigenvalues: 25.2997 29.6634 32.5371  
 58 H Isotropic = 27.2034 Anisotropy = 7.2632  
 XX= 30.6823 YX= -2.8041 ZX= 0.4386  
 XY= -1.6033 YY= 28.4829 ZY= -0.6357  
 XZ= -0.3541 YZ= 0.6468 ZZ= 22.4450  
 Eigenvalues: 22.4448 27.1199 32.0456  
 59 H Isotropic = 30.0885 Anisotropy = 5.9612  
 XX= 32.6177 YX= 1.3427 ZX= -2.0063  
 XY= 1.2954 YY= 28.7676 ZY= -2.0043  
 XZ= -1.3077 YZ= -2.2987 ZZ= 28.8801  
 Eigenvalues: 26.6626 29.5402 34.0626  
 60 H Isotropic = 29.6322 Anisotropy = 8.9697  
 XX= 27.9080 YX= -1.0907 ZX= -0.8813  
 XY= -1.1117 YY= 30.5113 ZY= 5.2021  
 XZ= -1.0468 YZ= 4.4794 ZZ= 30.4775  
 Eigenvalues: 25.6492 27.6355 35.6121  
 61 H Isotropic = 26.6313 Anisotropy = 2.3744  
 XX= 26.8364 YX= 0.7950 ZX= 1.9803  
 XY= 1.8728 YY= 26.6646 ZY= -0.4636  
 XZ= 0.9135 YZ= -1.7795 ZZ= 26.3928  
 Eigenvalues: 24.0228 27.6568 28.2142  
 62 H Isotropic = 30.7975 Anisotropy = 8.1858  
 XX= 30.3112 YX= 2.6568 ZX= -1.3151  
 XY= 2.8796 YY= 34.2179 ZY= -2.8348  
 XZ= -1.2348 YZ= -0.9041 ZZ= 27.8635  
 Eigenvalues: 27.2204 28.9175 36.2547  
 63 H Isotropic = 30.7436 Anisotropy = 7.6982  
 XX= 30.3854 YX= 1.2300 ZX= -0.9230  
 XY= 0.4269 YY= 32.3324 ZY= 4.5529  
 XZ= -2.2677 YZ= 4.9097 ZZ= 29.5131  
 Eigenvalues: 25.3587 30.9964 35.8758  
 64 H Isotropic = 30.6437 Anisotropy = 8.3357  
 XX= 34.7920 YX= -1.7259 ZX= 3.2566  
 XY= -0.1677 YY= 28.2888 ZY= 1.9893  
 XZ= 3.1794 YZ= 2.2440 ZZ= 28.8504  
 Eigenvalues: 25.5080 30.2222 36.2008  
 65 H Isotropic = 27.2825 Anisotropy = 7.2087  
 XX= 30.4146 YX= 2.8182 ZX= -0.5212  
 XY= 3.5787 YY= 25.9757 ZY= 0.4329  
 XZ= 0.0605 YZ= 0.4641 ZZ= 25.4571  
 Eigenvalues: 24.1129 25.6462 32.0883  
 66 H Isotropic = 29.4481 Anisotropy = 15.7558  
 XX= 34.4056 YX= -8.8094 ZX= 3.6229  
 XY= -6.7832 YY= 25.9786 ZY= 0.3357

XZ= 5.0898 YZ= 1.7466 ZZ= 27.9599  
 Eigenvalues: 20.0116 28.3807 39.9519  
 67 H Isotropic = 25.7685 Anisotropy = 13.5504  
 XX= 33.7729 YX= -2.8525 ZX= -1.1297  
 XY= -4.1688 YY= 21.9965 ZY= 0.1006  
 XZ= -0.7740 YZ= -0.1784 ZZ= 21.5361  
 Eigenvalues: 20.8866 21.6169 34.8021  
 68 H Isotropic = 29.7356 Anisotropy = 5.9308  
 XX= 31.6965 YX= 0.2718 ZX= 0.2066  
 XY= -1.5796 YY= 30.6114 ZY= -3.9186  
 XZ= 2.2083 YZ= -3.6199 ZZ= 26.8989  
 Eigenvalues: 24.4880 31.0293 33.6895  
 69 H Isotropic = 30.0783 Anisotropy = 7.5794  
 XX= 33.6029 YX= -0.9108 ZX= -2.9769  
 XY= -0.5387 YY= 30.5996 ZY= -1.1313  
 XZ= -4.4563 YZ= -1.3871 ZZ= 26.0324  
 Eigenvalues: 24.1892 30.9144 35.1312  
 70 H Isotropic = 30.4381 Anisotropy = 8.0273  
 XX= 29.5674 YX= 0.9050 ZX= 1.7093  
 XY= 1.4515 YY= 31.8333 ZY= 4.2868  
 XZ= 1.6814 YZ= 4.0628 ZZ= 29.9137  
 Eigenvalues: 26.4579 29.0668 35.7897  
 71 H Isotropic = 29.7604 Anisotropy = 6.4226  
 XX= 32.2057 YX= -3.5178 ZX= -1.7153  
 XY= -2.6048 YY= 28.9385 ZY= -2.7170  
 XZ= -2.3713 YZ= -4.1578 ZZ= 28.1368  
 Eigenvalues: 23.5874 31.6516 34.0421  
 72 H Isotropic = 29.6174 Anisotropy = 5.0091  
 XX= 30.0118 YX= -2.2550 ZX= 2.4422  
 XY= -3.2148 YY= 30.0999 ZY= 2.4025  
 XZ= 3.5473 YZ= 1.9414 ZZ= 28.7404  
 Eigenvalues: 24.2897 31.6057 32.9567  
 73 H Isotropic = 28.4521 Anisotropy = 3.2325  
 XX= 29.8687 YX= -0.6520 ZX= -1.6705  
 XY= -0.4485 YY= 29.8296 ZY= -0.6835  
 XZ= -1.3398 YZ= 0.1035 ZZ= 25.6581  
 Eigenvalues: 25.1331 29.6162 30.6072  
 74 H Isotropic = 30.3661 Anisotropy = 20.8160  
 XX= 35.6200 YX= -10.2778 ZX= 6.0082  
 XY= -9.4738 YY= 28.9124 ZY= -0.8741  
 XZ= 7.4010 YZ= 2.0717 ZZ= 26.5659  
 Eigenvalues: 18.9013 27.9535 44.2434  
 75 H Isotropic = 30.6103 Anisotropy = 8.4139  
 XX= 33.2188 YX= 3.4558 ZX= 0.9573  
 XY= 3.9408 YY= 31.6400 ZY= -0.7274  
 XZ= 0.4314 YZ= -1.8705 ZZ= 26.9721  
 Eigenvalues: 26.1325 29.4788 36.2196  
 76 H Isotropic = 30.1249 Anisotropy = 8.4578  
 XX= 29.3259 YX= -2.8800 ZX= -0.7572  
 XY= -3.5039 YY= 32.0887 ZY= -4.2180  
 XZ= -1.0029 YZ= -4.1330 ZZ= 28.9601  
 Eigenvalues: 24.5709 30.0404 35.7635  
 77 H Isotropic = 31.3846 Anisotropy = 7.6135  
 XX= 29.8128 YX= -1.6760 ZX= -3.2007  
 XY= -1.3236 YY= 29.4627 ZY= -0.8946

XZ= -3.2540 YZ= 0.0717 ZZ= 34.8783  
Eigenvalues: 27.2042 30.4893 36.4603

78 H Isotropic = 31.2551 Anisotropy = 8.7903  
XX= 32.3725 YX= 4.6184 ZX= -1.9783  
XY= 4.1298 YY= 32.5805 ZY= -1.2806  
XZ= -0.4335 YZ= -0.4969 ZZ= 28.8124  
Eigenvalues: 27.9981 28.6520 37.1153

79 H Isotropic = 31.3694 Anisotropy = 7.2012  
XX= 30.8713 YX= -0.2949 ZX= 1.1077  
XY= -0.7193 YY= 29.7718 ZY= 4.1372  
XZ= 0.7807 YZ= 4.0706 ZZ= 33.4651  
Eigenvalues: 26.8951 31.0430 36.1702

80 H Isotropic = 30.2225 Anisotropy = 9.2063  
XX= 33.6612 YX= -2.8607 ZX= 3.9536  
XY= -2.1599 YY= 28.7075 ZY= 0.8972  
XZ= 4.2710 YZ= 0.5734 ZZ= 28.2989  
Eigenvalues: 25.0534 29.2541 36.3601

81 H Isotropic = 27.6312 Anisotropy = 3.9469  
XX= 29.6950 YX= -0.0189 ZX= 1.3659  
XY= -1.9377 YY= 27.6411 ZY= 1.3620  
XZ= 1.5929 YZ= 1.9578 ZZ= 25.5574  
Eigenvalues: 24.0821 28.5489 30.2624

82 H Isotropic = 31.8788 Anisotropy = 18.9859  
XX= 28.5476 YX= -8.2363 ZX= -3.2031  
XY= -8.0215 YY= 35.8567 ZY= 6.5346  
XZ= -1.7637 YZ= 6.2676 ZZ= 31.2320  
Eigenvalues: 22.9551 28.1452 44.5361

83 H Isotropic = 31.0767 Anisotropy = 10.1276  
XX= 29.4934 YX= -2.6125 ZX= -3.8149  
XY= -1.6714 YY= 29.4237 ZY= 2.2686  
XZ= -4.0395 YZ= 2.9458 ZZ= 34.3129  
Eigenvalues: 27.0117 28.3899 37.8284

84 H Isotropic = 30.6806 Anisotropy = 6.5069  
XX= 32.1666 YX= 3.2302 ZX= -1.9140  
XY= 3.2130 YY= 29.9734 ZY= 1.0024  
XZ= -2.8383 YZ= 0.1655 ZZ= 29.9018  
Eigenvalues: 26.5343 30.4889 35.0185

85 H Isotropic = 30.2233 Anisotropy = 7.3078  
XX= 30.3207 YX= -3.6306 ZX= -0.0836  
XY= -4.0801 YY= 27.4085 ZY= -3.2317  
XZ= 0.0873 YZ= -3.0433 ZZ= 32.9407  
Eigenvalues: 23.9710 31.6038 35.0952

86 O Isotropic = -83.5767 Anisotropy = 607.6752  
XX= 198.9754 YX= -226.6026 ZX= 22.2172  
XY= -228.8517 YY= -103.3718 ZY= -18.3184  
XZ= 10.1570 YZ= 9.4038 ZZ= -346.3338  
Eigenvalues: -346.8493 -225.4209 321.5401

### Conformer 3

1 C Isotropic = 13.3790 Anisotropy = 87.6103  
XX= -77.8486 YX= -10.3983 ZX= 29.7146  
XY= -24.1062 YY= 63.5552 ZY= -2.6325  
XZ= 3.7539 YZ= -13.1702 ZZ= 54.4305  
Eigenvalues: -81.7354 50.0866 71.7859

2 C Isotropic = 65.0647 Anisotropy = 103.6065  
 XX= 88.4043 YX= 12.1533 ZX= -6.2720  
 XY= 19.6488 YY= 82.7137 ZY= -73.7071  
 XZ= -2.0546 YZ= -65.2931 ZZ= 24.0761  
 Eigenvalues: -22.2959 83.3543 134.1357

3 C Isotropic = 22.4136 Anisotropy = 206.7631  
 XX= 9.4990 YX= 60.1978 ZX= -15.6369  
 XY= 48.8934 YY= 67.1318 ZY= -101.8027  
 XZ= -21.0684 YZ= -106.6022 ZZ= -9.3901  
 Eigenvalues: -85.3514 -7.6635 160.2557

4 C Isotropic = 46.1252 Anisotropy = 121.4020  
 XX= 89.1455 YX= 15.1728 ZX= -34.8241  
 XY= 16.3745 YY= 64.9545 ZY= -65.4359  
 XZ= -36.0965 YZ= -61.1175 ZZ= -15.7244  
 Eigenvalues: -54.4478 65.7635 127.0599

5 C Isotropic = 41.5783 Anisotropy = 185.5793  
 XX= 82.1115 YX= 54.2295 ZX= -42.5837  
 XY= 43.6685 YY= 52.6595 ZY= -83.0569  
 XZ= -46.6416 YZ= -89.7706 ZZ= -10.0360  
 Eigenvalues: -71.1599 30.5970 165.2979

6 C Isotropic = 141.1416 Anisotropy = 22.0059  
 XX= 126.8429 YX= 1.0440 ZX= -13.7432  
 XY= 1.6133 YY= 155.3083 ZY= -0.4504  
 XZ= -6.7959 YZ= -3.0022 ZZ= 141.2736  
 Eigenvalues: 121.5030 146.1096 155.8122

7 C Isotropic = 109.9956 Anisotropy = 48.0200  
 XX= 109.6084 YX= -12.4176 ZX= -12.6665  
 XY= -13.9529 YY= 119.2150 ZY= 19.9202  
 XZ= -12.5921 YZ= 19.8439 ZZ= 101.1634  
 Eigenvalues: 87.5406 100.4373 142.0090

8 C Isotropic = 138.9875 Anisotropy = 40.4385  
 XX= 156.1212 YX= -2.1866 ZX= -22.3409  
 XY= -1.7085 YY= 130.6958 ZY= 7.6942  
 XZ= -13.2985 YZ= 7.2794 ZZ= 130.1455  
 Eigenvalues: 118.2594 132.7566 165.9465

9 C Isotropic = 34.1858 Anisotropy = 179.1884  
 XX= -23.2318 YX= 90.9137 ZX= 16.5970  
 XY= 92.4952 YY= 94.7494 ZY= -43.8035  
 XZ= 13.0459 YZ= -45.7926 ZZ= 31.0396  
 Eigenvalues: -84.0308 32.9434 153.6447

10 C Isotropic = 47.2401 Anisotropy = 109.7608  
 XX= 56.5990 YX= 19.8980 ZX= -33.3902  
 XY= 18.8602 YY= 83.0389 ZY= 65.8255  
 XZ= -37.0579 YZ= 67.1748 ZZ= 2.0823  
 Eigenvalues: -50.3953 71.7017 120.4140

11 C Isotropic = 42.5937 Anisotropy = 173.9109  
 XX= 10.7041 YX= 39.4105 ZX= -29.1614  
 XY= 41.5010 YY= 106.5988 ZY= 82.5826  
 XZ= -15.0211 YZ= 83.3305 ZZ= 10.4784  
 Eigenvalues: -60.0679 29.3147 158.5343

12 C Isotropic = 135.8291 Anisotropy = 39.8110  
 XX= 146.4587 YX= -22.0212 ZX= 11.7303  
 XY= -17.5307 YY= 126.9657 ZY= -8.8757  
 XZ= 6.8616 YZ= 0.5121 ZZ= 134.0629  
 Eigenvalues: 114.5575 130.5600 162.3698

13 C Isotropic = 106.0539 Anisotropy = 80.6837  
 XX= 127.2505 YX= -21.6975 ZX= 39.8010  
 XY= -18.8122 YY= 96.9152 ZY= -13.6688  
 XZ= 37.4724 YZ= -1.8414 ZZ= 93.9961  
 Eigenvalues: 67.6553 90.6634 159.8430

14 C Isotropic = 150.1377 Anisotropy = 30.9216  
 XX= 145.2860 YX= 0.2557 ZX= 2.5463  
 XY= 4.3844 YY= 165.2223 ZY= -13.8754  
 XZ= 17.2905 YZ= -11.8913 ZZ= 139.9048  
 Eigenvalues: 128.4761 151.1848 170.7521

15 C Isotropic = 104.7583 Anisotropy = 33.8360  
 XX= 122.0181 YX= 1.3324 ZX= -16.8260  
 XY= -6.8189 YY= 85.2940 ZY= -9.8617  
 XZ= -3.4496 YZ= -13.0743 ZZ= 106.9629  
 Eigenvalues: 79.3022 107.6571 127.3156

16 C Isotropic = 94.4914 Anisotropy = 63.2242  
 XX= 78.0424 YX= 6.2044 ZX= 14.8623  
 XY= 5.2234 YY= 129.2314 ZY= -17.3140  
 XZ= 7.3278 YZ= -24.8379 ZZ= 76.2005  
 Eigenvalues: 60.2445 86.5889 136.6409

17 C Isotropic = 113.0618 Anisotropy = 45.2995  
 XX= 93.7159 YX= 4.1745 ZX= 1.9848  
 XY= 10.4043 YY= 133.7457 ZY= -13.3572  
 XZ= 2.0301 YZ= -19.8277 ZZ= 111.7237  
 Eigenvalues: 90.8628 105.0611 143.2615

18 C Isotropic = 56.3076 Anisotropy = 125.9607  
 XX= -37.9584 YX= 31.7409 ZX= -11.6162  
 XY= 39.3032 YY= 71.5958 ZY= -23.7298  
 XZ= 9.5946 YZ= -10.9348 ZZ= 135.2854  
 Eigenvalues: -48.5538 77.1951 140.2814

19 C Isotropic = 37.7157 Anisotropy = 181.8431  
 XX= -67.9496 YX= 28.3685 ZX= 10.6165  
 XY= 23.5058 YY= 29.7313 ZY= -33.8351  
 XZ= -14.3122 YZ= -27.5470 ZZ= 151.3652  
 Eigenvalues: -74.5547 28.7573 158.9444

20 C Isotropic = 146.1975 Anisotropy = 24.9122  
 XX= 160.3911 YX= 11.4104 ZX= -0.2744  
 XY= 4.9958 YY= 134.8906 ZY= 4.1923  
 XZ= 0.7597 YZ= -3.9413 ZZ= 143.3108  
 Eigenvalues: 132.4794 143.3074 162.8056

21 C Isotropic = 103.8170 Anisotropy = 24.2006  
 XX= 119.4974 YX= -9.8803 ZX= 9.3133  
 XY= 7.4533 YY= 92.7148 ZY= -3.2140  
 XZ= -4.3721 YZ= -9.9307 ZZ= 99.2389  
 Eigenvalues: 88.6371 102.8632 119.9507

22 C Isotropic = 142.8560 Anisotropy = 20.8730  
 XX= 152.2540 YX= -1.3428 ZX= -6.0009  
 XY= 5.4895 YY= 132.3804 ZY= -0.1371  
 XZ= -8.8445 YZ= -0.8021 ZZ= 143.9336  
 Eigenvalues: 132.1568 139.6399 156.7713

23 C Isotropic = 113.5251 Anisotropy = 44.7641  
 XX= 134.4180 YX= 14.1539 ZX= -13.6810  
 XY= 19.6469 YY= 103.2150 ZY= 3.1291  
 XZ= -7.7298 YZ= 7.1313 ZZ= 102.9423  
 Eigenvalues: 89.3297 107.8779 143.3679

24 C Isotropic = 167.0887 Anisotropy = 27.8270  
XX= 162.6835 YX= 3.3755 ZX= -4.9115  
XY= 11.6511 YY= 176.8577 ZY= 11.6494  
XZ= -2.2801 YZ= 15.0075 ZZ= 161.7250  
Eigenvalues: 150.0208 165.6052 185.6400

25 C Isotropic = 171.8079 Anisotropy = 15.8755  
XX= 165.2951 YX= 12.8012 ZX= -0.1377  
XY= 12.2521 YY= 171.4986 ZY= 0.2093  
XZ= 4.8256 YZ= 1.2135 ZZ= 178.6300  
Eigenvalues: 155.4061 177.6261 182.3916

26 C Isotropic = 68.7373 Anisotropy = 144.5453  
XX= 18.2732 YX= 80.2857 ZX= 9.8327  
XY= 77.1756 YY= 105.9353 ZY= -47.1275  
XZ= 14.8985 YZ= -40.7204 ZZ= 82.0036  
Eigenvalues: -37.4913 78.6024 165.1009

27 C Isotropic = 168.1261 Anisotropy = 26.9241  
XX= 156.2879 YX= 2.7249 ZX= -0.5222  
XY= 7.5739 YY= 178.7357 ZY= -12.9453  
XZ= 4.2445 YZ= -8.3953 ZZ= 169.3547  
Eigenvalues: 153.7377 164.5651 186.0755

28 C Isotropic = 165.5275 Anisotropy = 30.7948  
XX= 175.6529 YX= -9.9444 ZX= -5.3987  
XY= -7.8785 YY= 169.3648 ZY= 4.9575  
XZ= -11.1838 YZ= 12.6289 ZZ= 151.5649  
Eigenvalues: 147.1711 163.3542 186.0574

29 C Isotropic = 161.0592 Anisotropy = 28.8554  
XX= 171.4318 YX= -11.4987 ZX= -5.3361  
XY= -15.2958 YY= 151.4268 ZY= 1.0710  
XZ= -5.5612 YZ= 6.4058 ZZ= 160.3190  
Eigenvalues: 144.6537 158.2278 180.2961

30 C Isotropic = 169.0994 Anisotropy = 31.7360  
XX= 152.4621 YX= -6.4472 ZX= 2.9364  
XY= -14.3426 YY= 185.5738 ZY= 8.1468  
XZ= -1.1141 YZ= 4.7241 ZZ= 169.2624  
Eigenvalues: 149.1031 167.9384 190.2568

31 C Isotropic = 170.5632 Anisotropy = 28.6198  
XX= 174.5504 YX= -15.4995 ZX= 5.1350  
XY= -11.5415 YY= 174.2220 ZY= -0.5245  
XZ= 9.9196 YZ= -3.4262 ZZ= 162.9172  
Eigenvalues: 157.2539 164.7926 189.6431

32 O Isotropic = 104.3795 Anisotropy = 131.1834  
XX= 155.6503 YX= 0.6242 ZX= 42.2432  
XY= 73.7626 YY= 124.5667 ZY= -118.4722  
XZ= 109.0060 YZ= -46.9968 ZZ= 32.9216  
Eigenvalues: -50.1738 171.4772 191.8351

33 O Isotropic = 255.9687 Anisotropy = 91.5838  
XX= 245.4029 YX= 3.1028 ZX= -28.9280  
XY= -17.0475 YY= 311.8223 ZY= -17.5446  
XZ= -18.3982 YZ= -29.2849 ZZ= 210.6810  
Eigenvalues: 193.7854 257.0962 317.0246

34 O Isotropic = 217.2962 Anisotropy = 91.6442  
XX= 229.1027 YX= 17.5523 ZX= 56.5440  
XY= 29.2843 YY= 259.3951 ZY= -10.9720  
XZ= 60.9202 YZ= -7.1901 ZZ= 163.3908  
Eigenvalues: 126.0065 247.4898 278.3923

35 O Isotropic = 281.9538 Anisotropy = 70.8625  
 XX= 302.0568 YX= 39.0651 ZX= 5.7592  
 XY= 26.3231 YY= 289.4380 ZY= -10.8314  
 XZ= 11.1617 YZ= 0.7944 ZZ= 254.3667  
 Eigenvalues: 248.2120 268.4540 329.1955  
 36 O Isotropic = 289.1764 Anisotropy = 59.7314  
 XX= 313.4044 YX= 14.1611 ZX= 17.3323  
 XY= 34.1034 YY= 284.3047 ZY= 7.0615  
 XZ= -0.1589 YZ= 6.3563 ZZ= 269.8203  
 Eigenvalues: 267.1401 271.3919 328.9974  
 37 O Isotropic = 266.0893 Anisotropy = 64.1145  
 XX= 249.4498 YX= 29.3131 ZX= -10.3927  
 XY= 23.2397 YY= 248.0337 ZY= 7.0710  
 XZ= -30.2993 YZ= -3.6176 ZZ= 300.7846  
 Eigenvalues: 219.4100 270.0257 308.8323  
 38 H Isotropic = 25.8225 Anisotropy = 8.8160  
 XX= 31.1268 YX= -1.3503 ZX= -1.0596  
 XY= -1.7970 YY= 23.7782 ZY= -2.2060  
 XZ= -2.5691 YZ= -0.7688 ZZ= 22.5625  
 Eigenvalues: 21.0011 24.7665 31.6998  
 39 H Isotropic = 30.1548 Anisotropy = 8.7481  
 XX= 34.6489 YX= 2.2150 ZX= -0.7369  
 XY= 3.6630 YY= 29.5005 ZY= 2.0664  
 XZ= -0.2679 YZ= 1.2149 ZZ= 26.3150  
 Eigenvalues: 25.3006 29.1770 35.9869  
 40 H Isotropic = 30.1741 Anisotropy = 6.0722  
 XX= 27.9587 YX= 0.3185 ZX= 0.0007  
 XY= -0.3870 YY= 31.0779 ZY= -3.1582  
 XZ= 1.5847 YZ= -2.5910 ZZ= 31.4858  
 Eigenvalues: 27.5797 28.7204 34.2223  
 41 H Isotropic = 27.8846 Anisotropy = 8.0541  
 XX= 30.5059 YX= -1.5351 ZX= 1.0750  
 XY= -3.3762 YY= 29.4429 ZY= 4.1605  
 XZ= -0.2195 YZ= 4.4348 ZZ= 23.7050  
 Eigenvalues: 21.1447 29.2551 33.2540  
 42 H Isotropic = 25.1824 Anisotropy = 6.4800  
 XX= 27.6176 YX= -2.5748 ZX= -1.6229  
 XY= -2.7060 YY= 25.7104 ZY= -2.3155  
 XZ= -2.0008 YZ= -1.3249 ZZ= 22.2191  
 Eigenvalues: 20.3642 25.6806 29.5024  
 43 H Isotropic = 25.3597 Anisotropy = 7.3665  
 XX= 26.8837 YX= -1.4876 ZX= -1.4013  
 XY= -2.3614 YY= 28.8832 ZY= -0.0780  
 XZ= -2.3045 YZ= 1.2158 ZZ= 20.3123  
 Eigenvalues: 19.8254 25.9830 30.2707  
 44 H Isotropic = 29.6569 Anisotropy = 3.8794  
 XX= 28.3009 YX= -1.8740 ZX= -1.4845  
 XY= -1.1682 YY= 28.5137 ZY= -0.1327  
 XZ= 0.3685 YZ= -0.6192 ZZ= 32.1560  
 Eigenvalues: 26.8000 29.9275 32.2431  
 45 H Isotropic = 28.7251 Anisotropy = 7.7662  
 XX= 33.2213 YX= 0.3960 ZX= -1.5633  
 XY= 1.5058 YY= 27.5657 ZY= -0.5963  
 XZ= -2.6593 YZ= 0.2066 ZZ= 25.3884  
 Eigenvalues: 24.8548 27.4180 33.9026

46 H Isotropic = 27.5521 Anisotropy = 3.7163  
 XX= 27.2112 YX= -2.4412 ZX= 0.1250  
 XY= -1.8501 YY= 26.0330 ZY= 2.0553  
 XZ= 0.8862 YZ= 0.9462 ZZ= 29.4121  
 Eigenvalues: 23.9789 28.6477 30.0297  
 47 H Isotropic = 31.4899 Anisotropy = 16.7995  
 XX= 25.6477 YX= -3.0340 ZX= -2.0739  
 XY= -3.1246 YY= 41.1263 ZY= -5.2374  
 XZ= -2.0139 YZ= -3.2083 ZZ= 27.6957  
 Eigenvalues: 23.0420 28.7382 42.6896  
 48 H Isotropic = 29.9094 Anisotropy = 3.9171  
 XX= 32.2781 YX= -0.4809 ZX= 0.5556  
 XY= -1.3450 YY= 28.3377 ZY= 1.6282  
 XZ= 0.4629 YZ= -0.4439 ZZ= 29.1124  
 Eigenvalues: 27.7748 29.4326 32.5208  
 49 H Isotropic = 29.6091 Anisotropy = 5.3543  
 XX= 28.4897 YX= 1.5374 ZX= -1.9569  
 XY= -1.1892 YY= 33.1704 ZY= 0.2381  
 XZ= -2.7870 YZ= 0.1227 ZZ= 27.1672  
 Eigenvalues: 25.3581 30.2905 33.1786  
 50 H Isotropic = 26.7253 Anisotropy = 5.4390  
 XX= 27.5022 YX= 1.8593 ZX= 3.9876  
 XY= 1.5929 YY= 25.0027 ZY= -0.5547  
 XZ= 1.2350 YZ= -0.3867 ZZ= 27.6710  
 Eigenvalues: 23.3659 26.4587 30.3513  
 51 H Isotropic = 26.5731 Anisotropy = 6.1616  
 XX= 24.7456 YX= 0.2607 ZX= -1.1549  
 XY= 0.6680 YY= 24.4245 ZY= 0.1804  
 XZ= 2.5414 YZ= -1.4102 ZZ= 30.5494  
 Eigenvalues: 23.9690 25.0695 30.6809  
 52 H Isotropic = 26.0100 Anisotropy = 9.3536  
 XX= 31.5562 YX= -0.2708 ZX= -2.9114  
 XY= -1.1630 YY= 25.7120 ZY= 1.1079  
 XZ= -2.2003 YZ= 0.3989 ZZ= 20.7618  
 Eigenvalues: 20.1268 25.6575 32.2457  
 53 H Isotropic = 30.5157 Anisotropy = 5.6383  
 XX= 28.1307 YX= -1.7852 ZX= 0.4354  
 XY= -1.6919 YY= 29.4527 ZY= 1.2299  
 XZ= -0.2368 YZ= 1.1410 ZZ= 33.9636  
 Eigenvalues: 26.8491 30.4234 34.2746  
 54 H Isotropic = 29.4624 Anisotropy = 6.9729  
 XX= 32.4555 YX= -1.9485 ZX= -0.7203  
 XY= -3.0179 YY= 28.8183 ZY= -3.3197  
 XZ= 0.6435 YZ= -3.4199 ZZ= 27.1134  
 Eigenvalues: 24.1780 30.0982 34.1110  
 55 H Isotropic = 30.4577 Anisotropy = 7.9486  
 XX= 32.4198 YX= 1.6885 ZX= 0.3376  
 XY= 4.1784 YY= 31.9210 ZY= -3.6628  
 XZ= -0.1738 YZ= -3.1041 ZZ= 27.0325  
 Eigenvalues: 25.0045 30.6119 35.7568  
 56 H Isotropic = 29.0670 Anisotropy = 4.7644  
 XX= 31.0721 YX= -2.3914 ZX= -0.0213  
 XY= -1.5328 YY= 28.9521 ZY= -0.6895  
 XZ= -1.2283 YZ= -1.1216 ZZ= 27.1770  
 Eigenvalues: 26.3402 28.6176 32.2433

57 H Isotropic = 29.0670 Anisotropy = 5.4747  
 XX= 31.3059 YX= -0.6823 ZX= 1.7122  
 XY= 0.4559 YY= 29.5900 ZY= 2.2777  
 XZ= 3.7743 YZ= 1.8287 ZZ= 26.3050  
 Eigenvalues: 24.3750 30.1092 32.7168  
 58 H Isotropic = 27.3398 Anisotropy = 6.4303  
 XX= 28.0873 YX= -1.7831 ZX= 1.2385  
 XY= -1.0242 YY= 26.9739 ZY= -3.6981  
 XZ= 0.0153 YZ= -4.4459 ZZ= 26.9582  
 Eigenvalues: 22.8340 27.5587 31.6267  
 59 H Isotropic = 29.9981 Anisotropy = 6.5302  
 XX= 33.3228 YX= 0.2677 ZX= 2.4853  
 XY= -0.0808 YY= 29.0978 ZY= -1.1110  
 XZ= 2.7875 YZ= -0.0382 ZZ= 27.5737  
 Eigenvalues: 26.4264 29.2164 34.3516  
 60 H Isotropic = 29.5907 Anisotropy = 8.7596  
 XX= 27.1351 YX= -0.6178 ZX= -1.7422  
 XY= -0.5068 YY= 26.7059 ZY= 1.1317  
 XZ= -0.9292 YZ= 1.8294 ZZ= 34.9312  
 Eigenvalues: 26.2807 27.0610 35.4304  
 61 H Isotropic = 26.6332 Anisotropy = 3.2459  
 XX= 28.5857 YX= -0.5721 ZX= -1.1518  
 XY= 1.4154 YY= 27.9559 ZY= 1.7347  
 XZ= -0.8746 YZ= 2.2884 ZZ= 23.3580  
 Eigenvalues: 22.4074 28.6950 28.7971  
 62 H Isotropic = 30.6416 Anisotropy = 10.1902  
 XX= 36.3362 YX= 3.5159 ZX= 0.3159  
 XY= 2.8442 YY= 28.0190 ZY= 2.3479  
 XZ= -1.1188 YZ= 2.8527 ZZ= 27.5695  
 Eigenvalues: 24.6383 29.8514 37.4350  
 63 H Isotropic = 31.0662 Anisotropy = 6.7141  
 XX= 31.5134 YX= -1.4009 ZX= -1.0069  
 XY= -1.2850 YY= 27.4807 ZY= 2.8039  
 XZ= -0.7670 YZ= 2.5032 ZZ= 34.2047  
 Eigenvalues: 26.3669 31.2896 35.5423  
 64 H Isotropic = 30.0577 Anisotropy = 9.1943  
 XX= 28.3148 YX= -3.2554 ZX= -0.6611  
 XY= -2.8904 YY= 34.9316 ZY= -0.4383  
 XZ= -1.2468 YZ= 1.1262 ZZ= 26.9266  
 Eigenvalues: 26.2241 27.7617 36.1872  
 65 H Isotropic = 26.6178 Anisotropy = 2.5714  
 XX= 26.9734 YX= 0.4210 ZX= 0.3227  
 XY= 0.3305 YY= 27.9146 ZY= 1.1760  
 XZ= 0.3491 YZ= 0.6678 ZZ= 24.9654  
 Eigenvalues: 24.6794 26.8419 28.3321  
 66 H Isotropic = 30.6502 Anisotropy = 16.4649  
 XX= 39.2719 YX= 4.7302 ZX= 1.9461  
 XY= 5.9085 YY= 29.5955 ZY= -4.3774  
 XZ= 2.2743 YZ= -4.1366 ZZ= 23.0831  
 Eigenvalues: 19.9793 30.3445 41.6268  
 67 H Isotropic = 25.9877 Anisotropy = 6.2308  
 XX= 25.7042 YX= 4.6342 ZX= 2.3108  
 XY= 2.5502 YY= 26.7473 ZY= -0.4993  
 XZ= 1.6918 YZ= -0.0483 ZZ= 25.5117  
 Eigenvalues: 21.7930 26.0286 30.1416

68 H Isotropic = 29.5021 Anisotropy = 7.1176  
XX= 34.0073 YX= 2.2001 ZX= 1.0206  
XY= -0.3730 YY= 27.5027 ZY= 3.1189  
XZ= -0.0669 YZ= 2.3209 ZZ= 26.9963  
Eigenvalues: 24.5105 29.7487 34.2472

69 H Isotropic = 30.2243 Anisotropy = 9.4302  
XX= 29.0339 YX= -0.7568 ZX= -0.6583  
XY= 0.3290 YY= 27.9480 ZY= 4.4768  
XZ= -0.2092 YZ= 5.2790 ZZ= 33.6912  
Eigenvalues: 25.1590 29.0029 36.5111

70 H Isotropic = 29.8609 Anisotropy = 2.1643  
XX= 30.2233 YX= -0.7453 ZX= -0.0820  
XY= 0.0135 YY= 30.5589 ZY= -0.8738  
XZ= -0.2742 YZ= -1.7257 ZZ= 28.8005  
Eigenvalues: 28.0600 30.2189 31.3038

71 H Isotropic = 29.8089 Anisotropy = 5.5053  
XX= 31.8833 YX= 3.6391 ZX= -1.2450  
XY= 2.1789 YY= 28.1758 ZY= 2.3359  
XZ= -1.6747 YZ= 2.8927 ZZ= 29.3677  
Eigenvalues: 24.6712 31.2764 33.4792

72 H Isotropic = 29.4341 Anisotropy = 6.0670  
XX= 31.7765 YX= -0.1418 ZX= 1.4296  
XY= 0.8469 YY= 26.8079 ZY= -3.5663  
XZ= 2.2286 YZ= -4.0750 ZZ= 29.7181  
Eigenvalues: 23.9434 30.8802 33.4788

73 H Isotropic = 28.2087 Anisotropy = 3.7885  
XX= 30.4379 YX= -0.0295 ZX= -1.1097  
XY= 1.0126 YY= 27.7295 ZY= 0.0737  
XZ= -0.8213 YZ= -0.0190 ZZ= 26.4585  
Eigenvalues: 26.2238 27.6678 30.7343

74 H Isotropic = 29.0370 Anisotropy = 28.5883  
XX= 41.4695 YX= 12.4268 ZX= 3.1175  
XY= 11.8675 YY= 24.6072 ZY= -0.3322  
XZ= 3.7244 YZ= -1.0933 ZZ= 21.0345  
Eigenvalues: 16.9681 22.0471 48.0959

75 H Isotropic = 30.6040 Anisotropy = 7.7128  
XX= 31.8019 YX= -1.9519 ZX= 1.3434  
XY= -3.0002 YY= 34.0213 ZY= -0.7853  
XZ= 1.1607 YZ= -0.1655 ZZ= 25.9887  
Eigenvalues: 25.7303 30.3357 35.7458

76 H Isotropic = 30.1162 Anisotropy = 8.7581  
XX= 30.5046 YX= 4.1297 ZX= -1.9643  
XY= 4.4046 YY= 32.5791 ZY= 1.2587  
XZ= -2.6495 YZ= 1.3125 ZZ= 27.2650  
Eigenvalues: 24.5915 29.8022 35.9550

77 H Isotropic = 31.2654 Anisotropy = 8.2513  
XX= 28.3681 YX= 1.4589 ZX= -0.4605  
XY= 0.9985 YY= 30.5646 ZY= 3.9721  
XZ= -0.7492 YZ= 2.8969 ZZ= 34.8635  
Eigenvalues: 27.1392 29.8907 36.7662

78 H Isotropic = 31.1422 Anisotropy = 8.5955  
XX= 29.9052 YX= -4.0490 ZX= 0.5018  
XY= -2.7304 YY= 35.2000 ZY= 0.3923  
XZ= 1.1715 YZ= -0.4670 ZZ= 28.3214  
Eigenvalues: 27.5418 29.0123 36.8726

79 H Isotropic = 31.3549 Anisotropy = 7.5262  
XX= 31.3749 YX= -0.6074 ZX= 1.8854  
XY= -0.6051 YY= 27.1411 ZY= -1.3928  
XZ= 1.5359 YZ= -1.1455 ZZ= 35.5487  
Eigenvalues: 26.9238 30.7685 36.3724

80 H Isotropic = 30.2773 Anisotropy = 9.6099  
XX= 36.4890 YX= 1.4445 ZX= 0.7223  
XY= 0.8340 YY= 26.1876 ZY= -1.5873  
XZ= 1.1638 YZ= -1.6387 ZZ= 28.1554  
Eigenvalues: 25.0960 29.0521 36.6839

81 H Isotropic = 27.6617 Anisotropy = 4.3821  
XX= 30.5346 YX= -0.8761 ZX= 0.0607  
XY= 0.9915 YY= 25.7542 ZY= -1.8861  
XZ= -0.7854 YZ= -1.9919 ZZ= 26.6963  
Eigenvalues: 24.2247 28.1772 30.5831

82 H Isotropic = 31.9035 Anisotropy = 18.7538  
XX= 30.1719 YX= 4.4075 ZX= -6.1560  
XY= 4.8391 YY= 25.7980 ZY= -4.6435  
XZ= -4.8150 YZ= -5.0061 ZZ= 39.7407  
Eigenvalues: 22.7614 28.5431 44.4061

83 H Isotropic = 31.1364 Anisotropy = 9.5154  
XX= 28.8340 YX= 1.1193 ZX= -2.5207  
XY= 0.3804 YY= 28.0467 ZY= 1.9219  
XZ= -2.6762 YZ= 1.0567 ZZ= 36.5285  
Eigenvalues: 26.8189 29.1104 37.4800

84 H Isotropic = 30.6233 Anisotropy = 5.9437  
XX= 29.4766 YX= -2.9408 ZX= -0.1603  
XY= -3.5256 YY= 32.3097 ZY= 0.2513  
XZ= -0.7320 YZ= 1.2107 ZZ= 30.0838  
Eigenvalues: 27.3630 29.9213 34.5858

85 H Isotropic = 30.4070 Anisotropy = 9.6961  
XX= 34.4072 YX= 4.3524 ZX= -0.6694  
XY= 4.9961 YY= 27.6410 ZY= 3.1700  
XZ= -0.9393 YZ= 3.1654 ZZ= 29.1729  
Eigenvalues: 23.4629 30.8871 36.8711

86 O Isotropic = -90.2974 Anisotropy = 612.6639  
XX= -232.7036 YX= -88.1905 ZX= 20.6012  
XY= -90.7183 YY= 79.4257 ZY= -293.3415  
XZ= 8.7963 YZ= -326.7242 ZZ= -117.6143  
Eigenvalues: -358.8252 -230.2122 318.1452

## Conformer 4

1 C Isotropic = 13.3400 Anisotropy = 87.6030  
XX= -45.9810 YX= 22.9946 ZX= -69.8250  
XY= 1.5279 YY= 52.2550 ZY= 9.1956  
XZ= -52.6370 YZ= 24.7209 ZZ= 33.7460  
Eigenvalues: -81.8455 50.1234 71.7420

2 C Isotropic = 64.9690 Anisotropy = 103.3473  
XX= 76.9696 YX= -24.2278 ZX= 14.3172  
XY= -19.2721 YY= 5.7830 ZY= 57.6573  
XZ= 13.0371 YZ= 46.7517 ZZ= 112.1545  
Eigenvalues: -22.0342 83.0741 133.8672

3 C Isotropic = 22.8441 Anisotropy = 206.2266  
XX= -5.7602 YX= 4.6808 ZX= 18.7962

XY= -5.5073 YY= -53.9528 ZY= 75.7680  
 XZ= 18.7588 YZ= 84.5737 ZZ= 128.2453  
 Eigenvalues: -84.8387 -6.9575 160.3285  
 4 C Isotropic = 46.0392 Anisotropy = 121.3395  
 XX= 50.3203 YX= -39.0750 ZX= 45.6029  
 XY= -40.3861 YY= -6.4494 ZY= 50.2863  
 XZ= 46.2019 YZ= 45.6769 ZZ= 94.2466  
 Eigenvalues: -54.6459 65.8312 126.9322  
 5 C Isotropic = 41.8209 Anisotropy = 184.8950  
 XX= 37.7070 YX= -17.4589 ZX= 58.8020  
 XY= -25.7902 YY= -41.2655 ZY= 48.4520  
 XZ= 57.8327 YZ= 58.4761 ZZ= 129.0211  
 Eigenvalues: -70.7385 31.1169 165.0842  
 6 C Isotropic = 141.3223 Anisotropy = 21.7014  
 XX= 122.0730 YX= -3.6443 ZX= 4.2986  
 XY= 1.2554 YY= 151.0748 ZY= 3.9047  
 XZ= -1.2246 YZ= 5.7750 ZZ= 150.8193  
 Eigenvalues: 121.9169 146.2602 155.7900  
 7 C Isotropic = 109.8641 Anisotropy = 48.0428  
 XX= 99.9475 YX= -10.7705 ZX= 8.0659  
 XY= -11.7906 YY= 137.1948 ZY= -7.2579  
 XZ= 7.5379 YZ= -6.4192 ZZ= 92.4501  
 Eigenvalues: 87.5419 100.1579 141.8927  
 8 C Isotropic = 138.6399 Anisotropy = 40.2263  
 XX= 139.8946 YX= -13.0315 ZX= 23.0219  
 XY= -8.0236 YY= 141.2224 ZY= -10.1495  
 XZ= 15.6422 YZ= -9.6530 ZZ= 134.8028  
 Eigenvalues: 117.8356 132.6267 165.4574  
 9 C Isotropic = 34.4553 Anisotropy = 179.2372  
 XX= -7.8903 YX= 72.2820 ZX= 5.4137  
 XY= 71.9769 YY= 8.0637 ZY= 71.8696  
 XZ= 9.1181 YZ= 73.1193 ZZ= 103.1926  
 Eigenvalues: -83.6811 33.1004 153.9468  
 10 C Isotropic = 47.6457 Anisotropy = 109.2726  
 XX= 22.5744 YX= 13.1716 ZX= 59.2180  
 XY= 10.3833 YY= 118.6279 ZY= -0.6936  
 XZ= 62.0284 YZ= -1.8024 ZZ= 1.7347  
 Eigenvalues: -49.7925 72.2354 120.4941  
 11 C Isotropic = 41.7089 Anisotropy = 175.0061  
 XX= -8.7240 YX= 43.0650 ZX= 54.6123  
 XY= 51.7005 YY= 141.0720 ZY= 11.3166  
 XZ= 43.5085 YZ= 9.2529 ZZ= -7.2214  
 Eigenvalues: -60.8319 27.5789 158.3796  
 12 C Isotropic = 135.7346 Anisotropy = 39.8110  
 XX= 151.5312 YX= -14.1185 ZX= -14.6570  
 XY= -16.8734 YY= 131.3517 ZY= 2.0545  
 XZ= -9.7494 YZ= -8.5092 ZZ= 124.3209  
 Eigenvalues: 114.0583 130.8702 162.2753  
 13 C Isotropic = 105.5095 Anisotropy = 79.9728  
 XX= 149.7235 YX= -6.9429 ZX= -24.8564  
 XY= -9.8523 YY= 89.0324 ZY= 17.2239  
 XZ= -23.1854 YZ= 4.6391 ZZ= 77.7726  
 Eigenvalues: 67.3198 90.3841 158.8247  
 14 C Isotropic = 150.2778 Anisotropy = 30.3807  
 XX= 151.3386 YX= -5.6236 ZX= -0.9937

XY= 5.3932 YY= 145.4087 ZY= 20.6941  
 XZ= -11.9784 YZ= 17.0742 ZZ= 154.0862  
 Eigenvalues: 129.6296 150.6722 170.5317  
 15 C Isotropic = 103.0493 Anisotropy = 31.5394  
 XX= 112.2507 YX= -11.5214 ZX= 13.1261  
 XY= -9.9491 YY= 82.3514 ZY= -11.8491  
 XZ= -1.1015 YZ= -6.0086 ZZ= 114.5458  
 Eigenvalues: 77.6312 107.4412 124.0756  
 16 C Isotropic = 95.5417 Anisotropy = 63.3917  
 XX= 86.1701 YX= 2.3144 ZX= -13.0028  
 XY= 0.9042 YY= 92.9304 ZY= 32.3403  
 XZ= -5.1296 YZ= 39.9406 ZZ= 107.5246  
 Eigenvalues: 61.3524 87.4700 137.8028  
 17 C Isotropic = 112.3611 Anisotropy = 42.4798  
 XX= 96.5967 YX= 2.3101 ZX= -8.4070  
 XY= 8.4081 YY= 108.4704 ZY= 14.5729  
 XZ= -1.8575 YZ= 18.5871 ZZ= 132.0161  
 Eigenvalues: 90.8914 105.5109 140.6809  
 18 C Isotropic = 52.8118 Anisotropy = 115.2458  
 XX= -14.6495 YX= 56.4069 ZX= -1.3722  
 XY= 56.2035 YY= 45.2997 ZY= -11.4028  
 XZ= 4.2448 YZ= -11.1600 ZZ= 127.7853  
 Eigenvalues: -48.7434 77.5365 129.6424  
 19 C Isotropic = 39.6811 Anisotropy = 175.4415  
 XX= -52.0715 YX= 41.9326 ZX= -12.4123  
 XY= 33.8608 YY= 28.4649 ZY= -37.4175  
 XZ= -8.1743 YZ= -39.7301 ZZ= 142.6499  
 Eigenvalues: -67.2103 29.6115 156.6421  
 20 C Isotropic = 144.1085 Anisotropy = 22.6201  
 XX= 159.1596 YX= -2.3702 ZX= -2.2065  
 XY= 1.3524 YY= 135.3732 ZY= -0.1481  
 XZ= 0.8435 YZ= -5.8313 ZZ= 137.7928  
 Eigenvalues: 133.3328 139.8042 159.1886  
 21 C Isotropic = 115.4389 Anisotropy = 32.1648  
 XX= 109.4895 YX= 9.1873 ZX= 1.2356  
 XY= 4.3019 YY= 111.6072 ZY= 13.2756  
 XZ= 3.5461 YZ= 18.4385 ZZ= 125.2201  
 Eigenvalues: 99.1794 110.2553 136.8821  
 22 C Isotropic = 143.4208 Anisotropy = 16.4301  
 XX= 145.4342 YX= 7.2709 ZX= 4.3133  
 XY= 2.6377 YY= 146.1402 ZY= 6.5921  
 XZ= 1.3001 YZ= 8.3257 ZZ= 138.6879  
 Eigenvalues: 134.0712 141.8169 154.3742  
 23 C Isotropic = 112.3679 Anisotropy = 49.1790  
 XX= 111.0371 YX= -19.1829 ZX= 0.6858  
 XY= -24.9304 YY= 128.6793 ZY= 9.4473  
 XZ= -3.6484 YZ= 9.1956 ZZ= 97.3873  
 Eigenvalues: 92.0366 99.9131 145.1539  
 24 C Isotropic = 166.6791 Anisotropy = 32.0786  
 XX= 185.9233 YX= 2.8538 ZX= 0.6689  
 XY= 10.8991 YY= 162.5640 ZY= 3.2595  
 XZ= 3.8426 YZ= 3.8675 ZZ= 151.5501  
 Eigenvalues: 150.4963 161.4763 188.0649  
 25 C Isotropic = 171.8854 Anisotropy = 15.7719  
 XX= 168.2816 YX= 12.4595 ZX= 2.8293

XY= 14.3049 YY= 169.4983 ZY= 0.8144  
 XZ= -1.8138 YZ= 0.2019 ZZ= 177.8762  
 Eigenvalues: 155.4939 177.7622 182.4000  
 26 C Isotropic = 69.0104 Anisotropy = 144.1067  
 XX= 33.3972 YX= 64.7312 ZX= 4.1931  
 XY= 61.9744 YY= 35.1314 ZY= 53.7641  
 XZ= -3.4173 YZ= 48.6973 ZZ= 138.5025  
 Eigenvalues: -36.8065 78.7561 165.0816  
 27 C Isotropic = 168.0497 Anisotropy = 27.0431  
 XX= 159.1379 YX= 1.3526 ZX= -3.9501  
 XY= 6.3043 YY= 164.9706 ZY= 14.0020  
 XZ= -6.2007 YZ= 7.8853 ZZ= 180.0406  
 Eigenvalues: 153.3129 164.7578 186.0784  
 28 C Isotropic = 165.9192 Anisotropy = 31.2216  
 XX= 166.9596 YX= -11.1482 ZX= 5.7793  
 XY= -14.2050 YY= 176.6480 ZY= 0.7933  
 XZ= 9.9210 YZ= -5.9233 ZZ= 154.1499  
 Eigenvalues: 149.9152 161.1088 186.7336  
 29 C Isotropic = 166.8069 Anisotropy = 19.5034  
 XX= 169.1208 YX= -7.5949 ZX= -1.5039  
 XY= -14.1275 YY= 168.6806 ZY= 2.1348  
 XZ= -2.2956 YZ= -3.5098 ZZ= 162.6193  
 Eigenvalues: 157.3982 163.2133 179.8091  
 30 C Isotropic = 168.8308 Anisotropy = 31.5935  
 XX= 169.4902 YX= 1.6847 ZX= -3.5076  
 XY= 1.2445 YY= 169.3007 ZY= -16.4297  
 XZ= -7.3693 YZ= -24.0181 ZZ= 167.7014  
 Eigenvalues: 147.8604 168.7388 189.8931  
 31 C Isotropic = 168.7972 Anisotropy = 31.2391  
 XX= 163.7646 YX= -14.0033 ZX= -2.4419  
 XY= -7.5905 YY= 183.3284 ZY= -10.2081  
 XZ= -3.2955 YZ= -6.8321 ZZ= 159.2985  
 Eigenvalues: 152.4299 164.3383 189.6232  
 32 O Isotropic = 102.7041 Anisotropy = 131.2132  
 XX= 188.5921 YX= -24.7588 ZX= 5.9161  
 XY= 45.6239 YY= 5.9116 ZY= 144.6047  
 XZ= -27.0112 YZ= 48.8308 ZZ= 113.6085  
 Eigenvalues: -51.7932 169.7258 190.1795  
 33 O Isotropic = 255.7066 Anisotropy = 92.3276  
 XX= 224.6738 YX= -27.1454 ZX= 25.2486  
 XY= -33.1464 YY= 271.1497 ZY= 36.0200  
 XZ= 7.8686 YZ= 53.7724 ZZ= 271.2963  
 Eigenvalues: 192.0757 257.7858 317.2583  
 34 O Isotropic = 220.3120 Anisotropy = 81.1368  
 XX= 258.1125 YX= 18.3865 ZX= -7.3046  
 XY= 25.8159 YY= 213.9152 ZY= 63.6770  
 XZ= -11.0058 YZ= 60.1791 ZZ= 188.9083  
 Eigenvalues: 134.6067 251.9261 274.4032  
 35 O Isotropic = 278.3976 Anisotropy = 73.3010  
 XX= 302.9137 YX= 23.4043 ZX= 30.7469  
 XY= 15.7678 YY= 258.6836 ZY= 28.1434  
 XZ= 12.8742 YZ= 21.7012 ZZ= 273.5957  
 Eigenvalues: 239.9715 267.9565 327.2650  
 36 O Isotropic = 279.7819 Anisotropy = 42.8078  
 XX= 298.7606 YX= -1.9667 ZX= -30.0595

XY= 9.2595 YY= 283.7587 ZY= 18.5440  
 XZ= -13.9702 YZ= -10.3440 ZZ= 256.8264  
 Eigenvalues: 246.6604 284.3649 308.3204  
 37 O Isotropic = 265.6623 Anisotropy = 61.1369  
 XX= 269.5650 YX= -1.0405 ZX= 8.3652  
 XY= -9.9298 YY= 263.3406 ZY= 33.8394  
 XZ= -0.4432 YZ= 51.5154 ZZ= 264.0812  
 Eigenvalues: 220.1279 270.4387 306.4202  
 38 H Isotropic = 25.8191 Anisotropy = 8.7093  
 XX= 28.9260 YX= -2.9640 ZX= 1.9325  
 XY= -4.5925 YY= 23.2062 ZY= 0.3224  
 XZ= 2.8796 YZ= -0.8007 ZZ= 25.3251  
 Eigenvalues: 21.1274 24.7046 31.6253  
 39 H Isotropic = 30.1623 Anisotropy = 8.6900  
 XX= 32.9391 YX= 0.4106 ZX= 4.2935  
 XY= 2.0614 YY= 29.4685 ZY= 0.5690  
 XZ= 4.7531 YZ= 0.8392 ZZ= 28.0793  
 Eigenvalues: 25.3743 29.1570 35.9557  
 40 H Isotropic = 30.1967 Anisotropy = 6.1240  
 XX= 29.0770 YX= -0.0162 ZX= -1.3966  
 XY= 0.0360 YY= 28.6165 ZY= 1.5918  
 XZ= -3.2401 YZ= 1.2311 ZZ= 32.8967  
 Eigenvalues: 27.5340 28.7768 34.2794  
 41 H Isotropic = 27.9185 Anisotropy = 8.0858  
 XX= 29.9643 YX= -0.6247 ZX= 1.3300  
 XY= -2.8400 YY= 32.3716 ZY= -0.1939  
 XZ= 1.4437 YZ= 0.2824 ZZ= 21.4195  
 Eigenvalues: 21.1910 29.2554 33.3090  
 42 H Isotropic = 25.1753 Anisotropy = 6.4865  
 XX= 25.8637 YX= -3.9451 ZX= 0.8611  
 XY= -4.6211 YY= 24.4439 ZY= 1.3513  
 XZ= 1.0310 YZ= 0.4695 ZZ= 25.2184  
 Eigenvalues: 20.4540 25.5724 29.4996  
 43 H Isotropic = 25.3933 Anisotropy = 7.3498  
 XX= 24.8083 YX= -2.5249 ZX= 2.0959  
 XY= -4.1338 YY= 28.1089 ZY= 2.7464  
 XZ= 2.1962 YZ= 1.8700 ZZ= 23.2627  
 Eigenvalues: 19.9202 25.9665 30.2932  
 44 H Isotropic = 29.6609 Anisotropy = 3.9120  
 XX= 28.5897 YX= -1.5997 ZX= -1.1161  
 XY= 0.0609 YY= 29.6387 ZY= -1.7731  
 XZ= -2.2163 YZ= -1.6637 ZZ= 30.7542  
 Eigenvalues: 26.8104 29.9034 32.2688  
 45 H Isotropic = 28.7431 Anisotropy = 7.7041  
 XX= 30.6679 YX= -1.4457 ZX= 3.3408  
 XY= -1.4172 YY= 27.1280 ZY= 0.7133  
 XZ= 4.6797 YZ= -0.4097 ZZ= 28.4334  
 Eigenvalues: 24.9202 27.4299 33.8791  
 46 H Isotropic = 27.5637 Anisotropy = 3.7496  
 XX= 27.9335 YX= -1.2028 ZX= -1.6153  
 XY= 0.0350 YY= 28.7176 ZY= -2.6497  
 XZ= -1.7662 YZ= -1.8434 ZZ= 26.0401  
 Eigenvalues: 23.9783 28.6495 30.0635  
 47 H Isotropic = 31.5417 Anisotropy = 16.7052  
 XX= 24.7331 YX= -3.9581 ZX= -1.5546

XY= -4.6771 YY= 35.1465 ZY= 7.5907  
 XZ= -1.9761 YZ= 5.7561 ZZ= 34.7456  
 Eigenvalues: 23.1310 28.8156 42.6785  
 48 H Isotropic = 29.8548 Anisotropy = 3.9490  
 XX= 32.2439 YX= -0.7747 ZX= 0.2442  
 XY= -0.8604 YY= 29.2688 ZY= -1.8809  
 XZ= 0.1567 YZ= 0.3809 ZZ= 28.0516  
 Eigenvalues: 27.6874 29.3895 32.4875  
 49 H Isotropic = 29.5834 Anisotropy = 5.3617  
 XX= 26.6603 YX= 0.2826 ZX= 2.1055  
 XY= -2.2777 YY= 32.0647 ZY= 1.2338  
 XZ= 1.5370 YZ= 2.4654 ZZ= 30.0253  
 Eigenvalues: 25.4300 30.1624 33.1579  
 50 H Isotropic = 26.7528 Anisotropy = 5.4143  
 XX= 29.2442 YX= 3.1600 ZX= -2.0706  
 XY= 1.4312 YY= 24.3985 ZY= 0.1208  
 XZ= 0.0955 YZ= 0.1420 ZZ= 26.6158  
 Eigenvalues: 23.4069 26.4892 30.3623  
 51 H Isotropic = 26.5622 Anisotropy = 6.2814  
 XX= 25.9888 YX= 0.1713 ZX= -0.7719  
 XY= 2.9089 YY= 25.0757 ZY= -2.4277  
 XZ= -3.4087 YZ= -1.2249 ZZ= 28.6222  
 Eigenvalues: 23.9066 25.0303 30.7499  
 52 H Isotropic = 26.0286 Anisotropy = 8.9563  
 XX= 28.2389 YX= -3.0704 ZX= 4.8083  
 XY= -3.1902 YY= 26.0689 ZY= -0.1232  
 XZ= 3.9183 YZ= 0.9057 ZZ= 23.7781  
 Eigenvalues: 20.3547 25.7317 31.9995  
 53 H Isotropic = 30.4731 Anisotropy = 5.9433  
 XX= 28.7021 YX= 0.3000 ZX= -2.7749  
 XY= 0.0583 YY= 32.1584 ZY= -2.4907  
 XZ= -2.1323 YZ= -2.4233 ZZ= 30.5587  
 Eigenvalues: 26.6734 30.3106 34.4353  
 54 H Isotropic = 29.4357 Anisotropy = 6.6678  
 XX= 31.5810 YX= -3.7801 ZX= 0.5061  
 XY= -3.8875 YY= 26.5151 ZY= 1.0941  
 XZ= -1.1633 YZ= 1.5699 ZZ= 30.2111  
 Eigenvalues: 24.2760 30.1502 33.8810  
 55 H Isotropic = 30.4341 Anisotropy = 8.1017  
 XX= 31.1903 YX= -0.2189 ZX= 1.3617  
 XY= 1.2752 YY= 27.1125 ZY= 4.4989  
 XZ= 2.9114 YZ= 3.0282 ZZ= 32.9995  
 Eigenvalues: 25.2392 30.2279 35.8352  
 56 H Isotropic = 28.9839 Anisotropy = 4.5900  
 XX= 29.8461 YX= -2.7534 ZX= -1.0122  
 XY= -2.5499 YY= 28.7072 ZY= 0.5141  
 XZ= 0.6595 YZ= 0.4733 ZZ= 28.3984  
 Eigenvalues: 26.5239 28.3839 32.0439  
 57 H Isotropic = 29.0531 Anisotropy = 5.1061  
 XX= 31.7633 YX= 0.1677 ZX= 0.2077  
 XY= 2.1695 YY= 30.4162 ZY= 1.4483  
 XZ= -0.9542 YZ= 1.2658 ZZ= 24.9798  
 Eigenvalues: 24.6028 30.0993 32.4572  
 58 H Isotropic = 27.3079 Anisotropy = 7.0037  
 XX= 27.2191 YX= -2.5271 ZX= -2.6724

XY= -2.3331 YY= 24.4175 ZY= 1.2194  
 XZ= -1.1028 YZ= 1.7292 ZZ= 30.2870  
 Eigenvalues: 22.9958 26.9508 31.9770  
 59 H Isotropic = 30.0068 Anisotropy = 6.1039  
 XX= 34.0724 YX= 0.1518 ZX= 0.1429  
 XY= -0.2873 YY= 27.9692 ZY= 1.7296  
 XZ= -0.3719 YZ= 0.9322 ZZ= 27.9788  
 Eigenvalues: 26.6429 29.3014 34.0760  
 60 H Isotropic = 29.6122 Anisotropy = 9.3562  
 XX= 26.8311 YX= 0.4615 ZX= -1.3207  
 XY= 0.8872 YY= 30.6481 ZY= -4.1338  
 XZ= -2.1440 YZ= -4.8648 ZZ= 31.3573  
 Eigenvalues: 25.8250 27.1619 35.8496  
 61 H Isotropic = 26.5856 Anisotropy = 3.2478  
 XX= 27.0738 YX= -1.2570 ZX= 1.9975  
 XY= 0.2014 YY= 28.5559 ZY= 1.1062  
 XZ= 2.7083 YZ= -0.0154 ZZ= 24.1271  
 Eigenvalues: 22.7320 28.2739 28.7508  
 62 H Isotropic = 30.5919 Anisotropy = 7.8655  
 XX= 34.6320 YX= 1.1547 ZX= 2.7238  
 XY= 0.0952 YY= 28.9305 ZY= -2.3193  
 XZ= 3.2951 YZ= -2.4077 ZZ= 28.2132  
 Eigenvalues: 25.3659 30.5743 35.8356  
 63 H Isotropic = 31.1208 Anisotropy = 7.7277  
 XX= 30.9200 YX= -0.8471 ZX= -0.9239  
 XY= -0.4264 YY= 32.1769 ZY= -5.0869  
 XZ= -1.0228 YZ= -4.8270 ZZ= 30.2656  
 Eigenvalues: 25.9064 31.1834 36.2726  
 64 H Isotropic = 30.1637 Anisotropy = 8.9659  
 XX= 28.0261 YX= -3.1103 ZX= -1.5983  
 XY= -3.4201 YY= 34.1021 ZY= 2.5438  
 XZ= -1.1926 YZ= 1.0091 ZZ= 28.3631  
 Eigenvalues: 26.3814 27.9688 36.1410  
 65 H Isotropic = 26.7383 Anisotropy = 3.1981  
 XX= 28.0401 YX= 0.9612 ZX= -0.6443  
 XY= 0.9534 YY= 27.6834 ZY= 0.7417  
 XZ= 0.1142 YZ= 1.0648 ZZ= 24.4915  
 Eigenvalues: 24.1852 27.1594 28.8704  
 66 H Isotropic = 30.3919 Anisotropy = 17.0458  
 XX= 39.8174 YX= 0.0901 ZX= 4.2456  
 XY= 1.1241 YY= 21.5144 ZY= 4.7515  
 XZ= 4.6563 YZ= 4.1071 ZZ= 29.8438  
 Eigenvalues: 19.5214 29.8985 41.7558  
 67 H Isotropic = 26.0749 Anisotropy = 9.8017  
 XX= 28.5311 YX= 5.2714 ZX= -0.5866  
 XY= 4.2485 YY= 26.6001 ZY= -0.6828  
 XZ= -1.3779 YZ= -1.1272 ZZ= 23.0934  
 Eigenvalues: 22.6815 22.9338 32.6094  
 68 H Isotropic = 29.6376 Anisotropy = 9.2387  
 XX= 35.5667 YX= 2.3923 ZX= 0.5608  
 XY= -0.2002 YY= 29.0077 ZY= -0.4288  
 XZ= 0.9407 YZ= 0.7871 ZZ= 24.3383  
 Eigenvalues: 24.2859 28.8301 35.7967  
 69 H Isotropic = 30.0093 Anisotropy = 7.4264  
 XX= 32.4176 YX= 0.9494 ZX= -1.9674

XY= 1.7704 YY= 32.8753 ZY= -1.7997  
 XZ= -2.1054 YZ= -2.8537 ZZ= 24.7350  
 Eigenvalues: 23.8000 31.2677 34.9603  
 70 H Isotropic = 30.1886 Anisotropy = 6.7927  
 XX= 30.3653 YX= 0.8458 ZX= -2.6511  
 XY= 1.2362 YY= 27.7415 ZY= 2.8827  
 XZ= -2.3148 YZ= 3.0632 ZZ= 32.4590  
 Eigenvalues: 25.4156 30.4331 34.7171  
 71 H Isotropic = 29.8509 Anisotropy = 6.1966  
 XX= 33.8590 YX= -0.0393 ZX= -0.2194  
 XY= 1.3534 YY= 29.9918 ZY= -3.0536  
 XZ= 0.8037 YZ= -3.8836 ZZ= 25.7019  
 Eigenvalues: 23.7359 31.8349 33.9820  
 72 H Isotropic = 29.2055 Anisotropy = 5.8856  
 XX= 31.8345 YX= 3.6492 ZX= -0.8688  
 XY= 2.5699 YY= 25.6294 ZY= 2.1274  
 XZ= -0.6599 YZ= 2.1121 ZZ= 30.1527  
 Eigenvalues: 23.5696 30.9178 33.1293  
 73 H Isotropic = 27.8961 Anisotropy = 3.1870  
 XX= 29.3820 YX= 0.1253 ZX= -0.0964  
 XY= -0.1539 YY= 29.5059 ZY= 1.2008  
 XZ= -0.8005 YZ= 1.9566 ZZ= 24.8005  
 Eigenvalues: 24.2845 29.3831 30.0208  
 74 H Isotropic = 30.3486 Anisotropy = 20.5790  
 XX= 40.6469 YX= 8.2975 ZX= 1.3733  
 XY= 8.7717 YY= 22.2608 ZY= 1.1585  
 XZ= -0.9894 YZ= 3.6124 ZZ= 28.1381  
 Eigenvalues: 18.4314 28.5465 44.0679  
 75 H Isotropic = 30.6354 Anisotropy = 8.6815  
 XX= 27.6037 YX= -1.2687 ZX= -0.3406  
 XY= -1.4182 YY= 34.3391 ZY= -2.8927  
 XZ= 0.3154 YZ= -4.0796 ZZ= 29.9635  
 Eigenvalues: 27.0236 28.4595 36.4231  
 76 H Isotropic = 31.2077 Anisotropy = 9.6791  
 XX= 35.2552 YX= 3.0863 ZX= -2.2304  
 XY= 3.1855 YY= 27.8969 ZY= -0.9645  
 XZ= -3.2665 YZ= -1.4553 ZZ= 30.4710  
 Eigenvalues: 26.7296 29.2331 37.6604  
 77 H Isotropic = 30.0934 Anisotropy = 7.3719  
 XX= 28.0391 YX= 3.2062 ZX= -0.3508  
 XY= 2.7469 YY= 27.3041 ZY= 0.5979  
 XZ= -0.6626 YZ= 0.7734 ZZ= 34.9369  
 Eigenvalues: 24.6026 30.6695 35.0080  
 78 H Isotropic = 31.3146 Anisotropy = 8.3412  
 XX= 30.6953 YX= -1.5835 ZX= 0.3853  
 XY= -0.5359 YY= 32.8873 ZY= -5.5665  
 XZ= -0.0154 YZ= -4.3249 ZZ= 30.3611  
 Eigenvalues: 26.4586 30.6098 36.8754  
 79 H Isotropic = 30.1084 Anisotropy = 7.6070  
 XX= 29.8441 YX= -1.7634 ZX= 0.2254  
 XY= -1.2612 YY= 32.1969 ZY= 4.6381  
 XZ= 0.6340 YZ= 3.9778 ZZ= 28.2841  
 Eigenvalues: 25.2017 29.9437 35.1797  
 80 H Isotropic = 31.3730 Anisotropy = 9.2357  
 XX= 37.1880 YX= -1.2263 ZX= -0.2951

XY= -1.8930 YY= 30.1478 ZY= 0.4927  
XZ= -0.2433 YZ= 0.4493 ZZ= 26.7834  
Eigenvalues: 26.7184 29.8706 37.5301

81 H Isotropic = 27.9545 Anisotropy = 2.1430  
XX= 28.3807 YX= 0.4974 ZX= 0.4778  
XY= 1.8897 YY= 27.3699 ZY= -1.4224  
XZ= -0.1149 YZ= -0.7220 ZZ= 28.1130  
Eigenvalues: 26.0781 28.4023 29.3832

82 H Isotropic = 32.0220 Anisotropy = 18.0432  
XX= 28.0551 YX= -1.2391 ZX= 1.0348  
XY= -0.9065 YY= 34.6585 ZY= 10.3923  
XZ= 1.4650 YZ= 9.6553 ZZ= 33.3524  
Eigenvalues: 23.3811 28.6342 44.0508

83 H Isotropic = 31.0447 Anisotropy = 9.9261  
XX= 30.4628 YX= 2.6984 ZX= 3.2110  
XY= 1.8590 YY= 29.0890 ZY= 4.0253  
XZ= 2.7289 YZ= 3.5634 ZZ= 33.5823  
Eigenvalues: 26.8040 28.6680 37.6621

84 H Isotropic = 30.4999 Anisotropy = 7.1338  
XX= 30.0160 YX= 4.7317 ZX= -0.8832  
XY= 4.0398 YY= 31.0138 ZY= -1.6030  
XZ= 0.0117 YZ= -0.9613 ZZ= 30.4700  
Eigenvalues: 26.0352 30.2088 35.2558

85 H Isotropic = 30.5031 Anisotropy = 9.1791  
XX= 35.4842 YX= -2.7306 ZX= 2.3957  
XY= -1.7697 YY= 29.5298 ZY= 1.5483  
XZ= 2.7113 YZ= 1.7241 ZZ= 26.4955  
Eigenvalues: 24.7817 30.1052 36.6226

86 O Isotropic = -92.0771 Anisotropy = 614.2258  
XX= -195.1372 YX= -146.5235 ZX= -166.5470  
XY= -146.2290 YY= -221.2466 ZY= 190.9030  
XZ= -152.1142 YZ= 221.9159 ZZ= 140.1526  
Eigenvalues: -362.2235 -231.4145 317.4067

## Conformer 5

1 C Isotropic = 13.3994 Anisotropy = 87.9266  
XX= -73.4725 YX= -11.4546 ZX= 40.7238  
XY= -26.5289 YY= 61.4835 ZY= -0.8210  
XZ= 16.2541 YZ= -13.1691 ZZ= 52.1873  
Eigenvalues: -81.6807 49.8619 72.0172

2 C Isotropic = 64.7895 Anisotropy = 103.7306  
XX= 86.5819 YX= 7.2423 ZX= -9.6656  
XY= 14.4703 YY= 72.3142 ZY= -78.2392  
XZ= -5.8354 YZ= -69.8468 ZZ= 35.4722  
Eigenvalues: -22.4100 82.8351 133.9432

3 C Isotropic = 22.8275 Anisotropy = 206.4821  
XX= 5.2551 YX= 50.0567 ZX= -18.0922  
XY= 38.7833 YY= 53.0023 ZY= -109.6116  
XZ= -22.5448 YZ= -115.2982 ZZ= 10.2251  
Eigenvalues: -84.8525 -7.1472 160.4822

4 C Isotropic = 46.6912 Anisotropy = 120.1412  
XX= 82.6975 YX= 7.0960 ZX= -41.4166  
XY= 8.1177 YY= 55.4774 ZY= -72.3579  
XZ= -42.5072 YZ= -67.3825 ZZ= 1.8988

Eigenvalues: -53.1824 66.4707 126.7853  
 5 C Isotropic = 42.6834 Anisotropy = 183.9398  
 XX= 74.0450 YX= 43.1059 ZX= -48.8418  
 XY= 33.8878 YY= 40.7952 ZY= -90.5821  
 XZ= -52.3587 YZ= -98.5160 ZZ= 13.2101  
 Eigenvalues: -69.9315 32.6718 165.3100  
 6 C Isotropic = 136.9162 Anisotropy = 28.5520  
 XX= 117.9931 YX= -1.2621 ZX= -12.7768  
 XY= -0.0869 YY= 154.7858 ZY= -1.5118  
 XZ= -5.0297 YZ= -7.3663 ZZ= 137.9697  
 Eigenvalues: 114.4781 140.3197 155.9509  
 7 C Isotropic = 110.1478 Anisotropy = 49.6255  
 XX= 105.8260 YX= -12.4815 ZX= -15.4265  
 XY= -14.1790 YY= 125.0924 ZY= 16.2925  
 XZ= -16.5885 YZ= 16.7256 ZZ= 99.5249  
 Eigenvalues: 85.6673 101.5445 143.2314  
 8 C Isotropic = 139.5884 Anisotropy = 41.9499  
 XX= 155.5284 YX= -1.9615 ZX= -23.8504  
 XY= -1.8224 YY= 129.6661 ZY= 9.5763  
 XZ= -14.4707 YZ= 7.1982 ZZ= 133.5706  
 Eigenvalues: 118.6173 132.5928 167.5550  
 9 C Isotropic = 34.2361 Anisotropy = 177.7157  
 XX= -23.9776 YX= 84.5873 ZX= 16.0178  
 XY= 86.6238 YY= 89.8541 ZY= -55.0049  
 XZ= 11.6437 YZ= -57.4896 ZZ= 36.8319  
 Eigenvalues: -83.3137 33.3088 152.7132  
 10 C Isotropic = 47.4271 Anisotropy = 108.9409  
 XX= 49.9640 YX= 20.8396 ZX= -41.1270  
 XY= 19.8532 YY= 94.0742 ZY= 55.4285  
 XZ= -44.6256 YZ= 57.0708 ZZ= -1.7567  
 Eigenvalues: -50.2139 72.4409 120.0544  
 11 C Isotropic = 42.1247 Anisotropy = 174.4133  
 XX= 3.6285 YX= 40.8840 ZX= -34.5890  
 XY= 43.7101 YY= 121.6731 ZY= 68.7976  
 XZ= -20.7909 YZ= 70.1906 ZZ= 1.0725  
 Eigenvalues: -60.6539 28.6277 158.4002  
 12 C Isotropic = 135.8079 Anisotropy = 39.7154  
 XX= 148.8932 YX= -20.1535 ZX= 12.7144  
 XY= -16.7579 YY= 125.6331 ZY= -6.5104  
 XZ= 7.4837 YZ= 3.0918 ZZ= 132.8974  
 Eigenvalues: 114.7358 130.4030 162.2849  
 13 C Isotropic = 105.9649 Anisotropy = 80.3017  
 XX= 134.0709 YX= -17.2810 ZX= 38.5544  
 XY= -15.3419 YY= 94.7802 ZY= -11.8975  
 XZ= 35.7065 YZ= 0.1700 ZZ= 89.0434  
 Eigenvalues: 67.7802 90.6151 159.4993  
 14 C Isotropic = 149.9931 Anisotropy = 30.2008  
 XX= 146.9134 YX= -1.0989 ZX= 2.6355  
 XY= 4.7710 YY= 162.2403 ZY= -15.9571  
 XZ= 16.8223 YZ= -13.5297 ZZ= 140.8256  
 Eigenvalues: 128.3884 151.4640 170.1270  
 15 C Isotropic = 104.2323 Anisotropy = 34.0014  
 XX= 120.4616 YX= -0.7000 ZX= -17.5816  
 XY= -6.9644 YY= 82.3925 ZY= -7.3813  
 XZ= -3.2683 YZ= -10.4952 ZZ= 109.8428

Eigenvalues: 78.6221 107.1749 126.8999  
 16 C Isotropic = 94.7592 Anisotropy = 62.9529  
 XX= 79.7736 YX= 5.1523 ZX= 14.5256  
 XY= 4.0309 YY= 124.2484 ZY= -22.6063  
 XZ= 7.6624 YZ= -30.4724 ZZ= 80.2554  
 Eigenvalues: 60.3679 87.1818 136.7278  
 17 C Isotropic = 112.6757 Anisotropy = 45.2239  
 XX= 93.6687 YX= 2.3170 ZX= 3.5371  
 XY= 8.8045 YY= 129.7640 ZY= -16.0672  
 XZ= 2.4126 YZ= -21.9541 ZZ= 114.5945  
 Eigenvalues: 90.6786 104.5236 142.8250  
 18 C Isotropic = 56.7665 Anisotropy = 124.5848  
 XX= -38.0286 YX= 29.7134 ZX= -3.7504  
 XY= 38.1932 YY= 70.5255 ZY= -18.8393  
 XZ= 15.7095 YZ= -4.8245 ZZ= 137.8027  
 Eigenvalues: -48.2119 78.6884 139.8231  
 19 C Isotropic = 36.2130 Anisotropy = 183.5539  
 XX= -69.2984 YX= 28.3595 ZX= 20.3627  
 XY= 20.2535 YY= 22.3030 ZY= -22.5692  
 XZ= -3.3038 YZ= -16.7431 ZZ= 155.6343  
 Eigenvalues: -76.0895 26.1462 158.5823  
 20 C Isotropic = 143.8527 Anisotropy = 31.8145  
 XX= 162.3102 YX= 13.0300 ZX= -2.2088  
 XY= 5.6238 YY= 133.1483 ZY= 2.4519  
 XZ= 1.0291 YZ= -4.3936 ZZ= 136.0995  
 Eigenvalues: 130.3186 136.1772 165.0623  
 21 C Isotropic = 105.1345 Anisotropy = 10.8423  
 XX= 112.0194 YX= -6.8553 ZX= -1.2132  
 XY= 3.4780 YY= 95.4232 ZY= -3.4747  
 XZ= -1.2188 YZ= -10.2910 ZZ= 107.9608  
 Eigenvalues: 92.1733 110.8675 112.3627  
 22 C Isotropic = 143.0359 Anisotropy = 11.8658  
 XX= 150.7606 YX= -5.4450 ZX= 3.2342  
 XY= 2.6652 YY= 137.8960 ZY= 0.3354  
 XZ= -2.3897 YZ= -4.0877 ZZ= 140.4512  
 Eigenvalues: 136.8261 141.3352 150.9465  
 23 C Isotropic = 107.6817 Anisotropy = 42.3112  
 XX= 97.6007 YX= -3.8624 ZX= 4.4851  
 XY= -6.1986 YY= 90.0518 ZY= 0.6294  
 XZ= 4.2011 YZ= 1.3539 ZZ= 135.3927  
 Eigenvalues: 87.3673 99.7887 135.8892  
 24 C Isotropic = 166.7563 Anisotropy = 27.2059  
 XX= 154.5123 YX= -4.7300 ZX= 0.0434  
 XY= -2.0338 YY= 184.0597 ZY= 7.5403  
 XZ= 1.9719 YZ= -0.8058 ZZ= 161.6970  
 Eigenvalues: 153.8758 161.4996 184.8936  
 25 C Isotropic = 172.0095 Anisotropy = 15.6802  
 XX= 165.1216 YX= 12.8395 ZX= -0.2501  
 XY= 12.4053 YY= 172.3512 ZY= -0.2247  
 XZ= 4.8486 YZ= 0.5271 ZZ= 178.5558  
 Eigenvalues: 155.4742 178.0914 182.4630  
 26 C Isotropic = 68.7836 Anisotropy = 145.1880  
 XX= 16.5321 YX= 74.8940 ZX= 9.3791  
 XY= 71.1856 YY= 101.5751 ZY= -56.7841  
 XZ= 15.0984 YZ= -48.0110 ZZ= 88.2437

Eigenvalues: -37.0204 77.7956 165.5756  
 27 C Isotropic = 168.1093 Anisotropy = 26.8429  
 XX= 156.2856 YX= 1.5602 ZX= 0.7346  
 XY= 6.4322 YY= 177.1271 ZY= -14.0581  
 XZ= 5.0234 YZ= -8.9441 ZZ= 170.9152  
 Eigenvalues: 153.6073 164.7161 186.0046  
 28 C Isotropic = 165.5958 Anisotropy = 30.8855  
 XX= 174.9371 YX= -9.7156 ZX= -5.7478  
 XY= -9.0125 YY= 170.6463 ZY= 3.7206  
 XZ= -11.7742 YZ= 11.2292 ZZ= 151.2040  
 Eigenvalues: 147.4084 163.1929 186.1862  
 29 C Isotropic = 160.8905 Anisotropy = 28.9226  
 XX= 171.3477 YX= -11.2472 ZX= -4.6027  
 XY= -15.5369 YY= 151.9090 ZY= 2.7615  
 XZ= -4.5271 YZ= 7.5538 ZZ= 159.4147  
 Eigenvalues: 144.6129 157.8864 180.1722  
 30 C Isotropic = 159.3033 Anisotropy = 40.2251  
 XX= 145.6992 YX= 1.8724 ZX= -10.6323  
 XY= 4.4210 YY= 151.1376 ZY= 7.5601  
 XZ= -11.4447 YZ= 10.9630 ZZ= 181.0732  
 Eigenvalues: 139.4906 152.2994 186.1201  
 31 C Isotropic = 168.8905 Anisotropy = 25.6780  
 XX= 163.4997 YX= 0.9470 ZX= -1.0601  
 XY= -2.7798 YY= 184.9921 ZY= 7.5211  
 XZ= -4.5014 YZ= 2.6310 ZZ= 158.1796  
 Eigenvalues: 156.3217 164.3405 186.0092  
 32 O Isotropic = 103.6445 Anisotropy = 129.7946  
 XX= 162.6023 YX= 0.3396 ZX= 35.4514  
 XY= 74.8489 YY= 110.5343 ZY= -130.8798  
 XZ= 93.9955 YZ= -52.7120 ZZ= 37.7969  
 Eigenvalues: -50.7198 171.4791 190.1742  
 33 O Isotropic = 244.1782 Anisotropy = 35.2146  
 XX= 238.0376 YX= -5.0760 ZX= -3.9905  
 XY= -15.8750 YY= 259.8238 ZY= 5.2818  
 XZ= -7.7440 YZ= 13.4827 ZZ= 234.6731  
 Eigenvalues: 230.1488 234.7311 267.6546  
 34 O Isotropic = 216.9133 Anisotropy = 90.9630  
 XX= 237.1334 YX= 21.6632 ZX= 48.3627  
 XY= 32.8690 YY= 256.3512 ZY= -22.8169  
 XZ= 51.2672 YZ= -18.6456 ZZ= 157.2554  
 Eigenvalues: 126.1084 247.0762 277.5553  
 35 O Isotropic = 281.7443 Anisotropy = 70.7520  
 XX= 301.1488 YX= 39.4216 ZX= -1.0229  
 XY= 26.7888 YY= 288.6579 ZY= -16.0822  
 XZ= 6.0763 YZ= -5.0598 ZZ= 255.4263  
 Eigenvalues: 247.9645 268.3561 328.9123  
 36 O Isotropic = 286.7833 Anisotropy = 48.0651  
 XX= 307.2336 YX= 16.2288 ZX= 10.5060  
 XY= 26.3990 YY= 278.1084 ZY= -1.9155  
 XZ= -14.9179 YZ= -6.2870 ZZ= 275.0080  
 Eigenvalues: 266.0771 275.4462 318.8267  
 37 O Isotropic = 256.9471 Anisotropy = 66.1303  
 XX= 261.1207 YX= -19.1913 ZX= 39.0724  
 XY= -23.8524 YY= 245.7971 ZY= -8.5459  
 XZ= 28.7252 YZ= 6.9974 ZZ= 263.9235

Eigenvalues: 219.0802 250.7271 301.0340  
 38 H Isotropic = 25.8143 Anisotropy = 8.7802  
 XX= 30.8713 YX= -1.3856 ZX= -1.4544  
 XY= -2.0399 YY= 23.4543 ZY= -2.1215  
 XZ= -2.9741 YZ= -0.8157 ZZ= 23.1172  
 Eigenvalues: 21.0155 24.7597 31.6677  
 39 H Isotropic = 30.1939 Anisotropy = 8.8663  
 XX= 34.3610 YX= 2.4578 ZX= -1.5642  
 XY= 3.9556 YY= 29.9539 ZY= 1.4634  
 XZ= -1.2154 YZ= 0.6707 ZZ= 26.2667  
 Eigenvalues: 25.3486 29.1284 36.1048  
 40 H Isotropic = 30.2015 Anisotropy = 6.1864  
 XX= 28.0661 YX= 0.0573 ZX= 0.3319  
 XY= -0.6002 YY= 30.8341 ZY= -3.0764  
 XZ= 2.0549 YZ= -2.5927 ZZ= 31.7043  
 Eigenvalues: 27.5192 28.7595 34.3258  
 41 H Isotropic = 27.8830 Anisotropy = 8.1658  
 XX= 30.7087 YX= -1.2407 ZX= 0.5502  
 XY= -3.2187 YY= 29.8459 ZY= 3.9645  
 XZ= -0.5500 YZ= 4.0826 ZZ= 23.0944  
 Eigenvalues: 21.1215 29.2006 33.3268  
 42 H Isotropic = 25.2667 Anisotropy = 6.4228  
 XX= 27.4579 YX= -2.7736 ZX= -1.7985  
 XY= -3.0324 YY= 25.3972 ZY= -2.4118  
 XZ= -2.0956 YZ= -1.4757 ZZ= 22.9451  
 Eigenvalues: 20.4147 25.8368 29.5486  
 43 H Isotropic = 25.3996 Anisotropy = 7.2296  
 XX= 26.7795 YX= -1.5619 ZX= -1.7205  
 XY= -2.5523 YY= 28.7883 ZY= -0.5462  
 XZ= -2.5954 YZ= 0.5371 ZZ= 20.6309  
 Eigenvalues: 19.9027 26.0767 30.2193  
 44 H Isotropic = 30.0300 Anisotropy = 3.5601  
 XX= 28.7345 YX= -2.2004 ZX= -1.4419  
 XY= -1.1744 YY= 29.0513 ZY= 0.0580  
 XZ= 0.3315 YZ= -0.1741 ZZ= 32.3043  
 Eigenvalues: 27.1585 30.5281 32.4034  
 45 H Isotropic = 28.6206 Anisotropy = 7.2259  
 XX= 32.4704 YX= 0.3090 ZX= -1.9320  
 XY= 1.4070 YY= 27.4715 ZY= -0.7965  
 XZ= -3.0143 YZ= 0.1929 ZZ= 25.9200  
 Eigenvalues: 25.0910 27.3330 33.4379  
 46 H Isotropic = 27.8217 Anisotropy = 3.0321  
 XX= 27.7618 YX= -1.8530 ZX= 0.2890  
 XY= -1.6909 YY= 26.4222 ZY= 1.8838  
 XZ= 1.0876 YZ= 0.8875 ZZ= 29.2811  
 Eigenvalues: 24.6861 28.9358 29.8431  
 47 H Isotropic = 31.5748 Anisotropy = 13.3049  
 XX= 28.2844 YX= -1.5169 ZX= 2.7833  
 XY= -1.3803 YY= 30.4141 ZY= 6.6816  
 XZ= 2.8162 YZ= 6.1849 ZZ= 36.0259  
 Eigenvalues: 24.2571 30.0225 40.4448  
 48 H Isotropic = 30.2923 Anisotropy = 4.1836  
 XX= 32.9103 YX= -0.5515 ZX= 0.1818  
 XY= -1.1656 YY= 28.7732 ZY= 1.9586  
 XZ= 0.1538 YZ= -0.2828 ZZ= 29.1935

Eigenvalues: 27.9936 29.8021 33.0814  
 49 H Isotropic = 29.0896 Anisotropy = 5.4631  
 XX= 27.4777 YX= 1.3318 ZX= -2.1598  
 XY= -1.3641 YY= 32.6960 ZY= -0.1369  
 XZ= -2.5808 YZ= -0.6845 ZZ= 27.0952  
 Eigenvalues: 24.8959 29.6414 32.7317  
 50 H Isotropic = 26.7132 Anisotropy = 5.4483  
 XX= 27.8503 YX= 2.1815 ZX= 3.7953  
 XY= 1.7678 YY= 24.9573 ZY= -0.4503  
 XZ= 1.0967 YZ= -0.3527 ZZ= 27.3321  
 Eigenvalues: 23.3070 26.4873 30.3454  
 51 H Isotropic = 26.4941 Anisotropy = 6.1338  
 XX= 24.7996 YX= 0.0820 ZX= -0.6921  
 XY= 0.9290 YY= 24.3229 ZY= 0.6722  
 XZ= 2.9653 YZ= -0.8591 ZZ= 30.3600  
 Eigenvalues: 23.9201 24.9790 30.5833  
 52 H Isotropic = 26.0829 Anisotropy = 9.2899  
 XX= 31.1734 YX= -0.4284 ZX= -3.7022  
 XY= -1.1848 YY= 25.8943 ZY= 0.8192  
 XZ= -2.8502 YZ= 0.0065 ZZ= 21.1811  
 Eigenvalues: 20.1979 25.7747 32.2762  
 53 H Isotropic = 30.4841 Anisotropy = 5.7048  
 XX= 28.1661 YX= -1.6098 ZX= 1.0173  
 XY= -1.5789 YY= 29.6291 ZY= 1.7666  
 XZ= 0.3670 YZ= 1.6545 ZZ= 33.6572  
 Eigenvalues: 26.7979 30.3671 34.2874  
 54 H Isotropic = 29.4310 Anisotropy = 6.9226  
 XX= 32.5050 YX= -2.1675 ZX= -0.8985  
 XY= -3.1043 YY= 28.0945 ZY= -3.2084  
 XZ= 0.6012 YZ= -3.3484 ZZ= 27.6935  
 Eigenvalues: 24.1450 30.1019 34.0461  
 55 H Isotropic = 30.4492 Anisotropy = 7.9993  
 XX= 32.1748 YX= 1.4756 ZX= -0.1135  
 XY= 3.8938 YY= 31.4132 ZY= -4.3838  
 XZ= -0.8105 YZ= -3.6185 ZZ= 27.7597  
 Eigenvalues: 25.0131 30.5525 35.7821  
 56 H Isotropic = 29.0496 Anisotropy = 4.8151  
 XX= 31.0272 YX= -2.4703 ZX= 0.0161  
 XY= -1.7077 YY= 28.7154 ZY= -0.6715  
 XZ= -1.1944 YZ= -1.0702 ZZ= 27.4061  
 Eigenvalues: 26.3945 28.4945 32.2597  
 57 H Isotropic = 29.0546 Anisotropy = 5.5815  
 XX= 31.6066 YX= -0.2789 ZX= 1.4121  
 XY= 1.0108 YY= 29.9217 ZY= 1.8639  
 XZ= 3.3907 YZ= 1.5499 ZZ= 25.6355  
 Eigenvalues: 24.3821 30.0061 32.7756  
 58 H Isotropic = 27.3243 Anisotropy = 6.5231  
 XX= 28.0326 YX= -1.9772 ZX= 1.4111  
 XY= -1.2549 YY= 26.2669 ZY= -3.5170  
 XZ= 0.1771 YZ= -4.2494 ZZ= 27.6734  
 Eigenvalues: 22.9119 27.3879 31.6730  
 59 H Isotropic = 29.9772 Anisotropy = 6.5271  
 XX= 33.6114 YX= 0.5646 ZX= 2.0691  
 XY= 0.1970 YY= 28.9731 ZY= -1.1700  
 XZ= 2.3896 YZ= -0.1643 ZZ= 27.3472

Eigenvalues: 26.4139 29.1892 34.3286  
 60 H Isotropic = 29.6029 Anisotropy = 8.9311  
 XX= 26.8693 YX= -0.6398 ZX= -1.1442  
 XY= -0.5121 YY= 27.0903 ZY= 1.9215  
 XZ= -0.2748 YZ= 2.6654 ZZ= 34.8491  
 Eigenvalues: 26.2247 27.0271 35.5570  
 61 H Isotropic = 26.6274 Anisotropy = 3.2761  
 XX= 28.4356 YX= -0.6144 ZX= -1.4917  
 XY= 1.3444 YY= 28.2480 ZY= 1.1963  
 XZ= -1.3824 YZ= 1.9088 ZZ= 23.1986  
 Eigenvalues: 22.3957 28.6750 28.8114  
 62 H Isotropic = 30.6188 Anisotropy = 9.6890  
 XX= 36.0112 YX= 3.4200 ZX= -0.2251  
 XY= 2.6081 YY= 28.5613 ZY= 2.3359  
 XZ= -1.4780 YZ= 2.7824 ZZ= 27.2839  
 Eigenvalues: 24.6905 30.0878 37.0782  
 63 H Isotropic = 31.1066 Anisotropy = 7.0089  
 XX= 31.3236 YX= -1.4202 ZX= -0.6251  
 XY= -1.2683 YY= 28.1350 ZY= 3.6449  
 XZ= -0.3818 YZ= 3.3920 ZZ= 33.8612  
 Eigenvalues: 26.2607 31.2799 35.7792  
 64 H Isotropic = 30.0641 Anisotropy = 9.1241  
 XX= 28.4155 YX= -3.4789 ZX= -0.1753  
 XY= -3.2602 YY= 34.6781 ZY= -0.9653  
 XZ= -0.8608 YZ= 0.6052 ZZ= 27.0988  
 Eigenvalues: 26.4707 27.5748 36.1469  
 65 H Isotropic = 26.5989 Anisotropy = 2.4708  
 XX= 27.0438 YX= 0.3193 ZX= 0.2584  
 XY= 0.3500 YY= 28.0350 ZY= 0.8695  
 XZ= 0.2698 YZ= 0.2634 ZZ= 24.7180  
 Eigenvalues: 24.6063 26.9444 28.2461  
 66 H Isotropic = 30.6682 Anisotropy = 16.5522  
 XX= 39.4469 YX= 4.6790 ZX= 0.7402  
 XY= 5.9310 YY= 28.6494 ZY= -5.2893  
 XZ= 0.9222 YZ= -4.9876 ZZ= 23.9085  
 Eigenvalues: 19.9230 30.3787 41.7030  
 67 H Isotropic = 25.9946 Anisotropy = 7.0590  
 XX= 26.5055 YX= 5.0815 ZX= 1.9786  
 XY= 2.8527 YY= 26.6397 ZY= -0.5091  
 XZ= 1.5730 YZ= -0.3345 ZZ= 24.8386  
 Eigenvalues: 21.7798 25.5034 30.7006  
 68 H Isotropic = 29.5325 Anisotropy = 7.3508  
 XX= 34.1711 YX= 2.5029 ZX= 0.4437  
 XY= -0.1047 YY= 28.0614 ZY= 3.0340  
 XZ= -0.3796 YZ= 2.0111 ZZ= 26.3651  
 Eigenvalues: 24.5041 29.6604 34.4331  
 69 H Isotropic = 30.1928 Anisotropy = 9.0925  
 XX= 29.2286 YX= -0.4543 ZX= -0.3336  
 XY= 0.5588 YY= 28.9441 ZY= 4.8724  
 XZ= -0.0639 YZ= 5.7312 ZZ= 32.4057  
 Eigenvalues: 25.0916 29.2323 36.2545  
 70 H Isotropic = 29.8536 Anisotropy = 2.2580  
 XX= 30.3669 YX= -0.8087 ZX= 0.1058  
 XY= -0.0740 YY= 30.2303 ZY= -1.0913  
 XZ= -0.1627 YZ= -1.9222 ZZ= 28.9638

Eigenvalues: 27.9326 30.2693 31.3590  
 71 H Isotropic = 29.7265 Anisotropy = 6.0178  
 XX= 32.5490 YX= 3.3595 ZX= -1.4359  
 XY= 1.5314 YY= 28.4628 ZY= 2.4292  
 XZ= -1.9580 YZ= 2.7829 ZZ= 28.1676  
 Eigenvalues: 24.6259 30.8152 33.7384  
 72 H Isotropic = 29.0732 Anisotropy = 7.0355  
 XX= 33.1498 YX= 0.1016 ZX= 1.5039  
 XY= 0.9785 YY= 25.4686 ZY= -2.3985  
 XZ= 1.9821 YZ= -3.2482 ZZ= 28.6014  
 Eigenvalues: 23.6106 29.8455 33.7636  
 73 H Isotropic = 28.0748 Anisotropy = 5.5452  
 XX= 31.5774 YX= -1.0471 ZX= 0.9313  
 XY= 0.1616 YY= 28.5052 ZY= -0.7867  
 XZ= 0.8604 YZ= -0.7493 ZZ= 24.1420  
 Eigenvalues: 23.9245 28.5284 31.7716  
 74 H Isotropic = 29.0679 Anisotropy = 27.4423  
 XX= 40.6805 YX= 12.5423 ZX= 1.1100  
 XY= 11.9264 YY= 24.9606 ZY= -1.5676  
 XZ= 1.5041 YZ= -2.7354 ZZ= 21.5624  
 Eigenvalues: 16.9174 22.9234 47.3627  
 75 H Isotropic = 31.0104 Anisotropy = 7.5036  
 XX= 28.5601 YX= -0.7670 ZX= -0.9373  
 XY= -0.4682 YY= 32.2422 ZY= 2.8155  
 XZ= -0.8836 YZ= 4.4255 ZZ= 32.2288  
 Eigenvalues: 28.2777 28.7406 36.0128  
 76 H Isotropic = 31.3147 Anisotropy = 10.0394  
 XX= 33.2068 YX= 1.9430 ZX= -4.0503  
 XY= 2.0356 YY= 28.2708 ZY= -0.9052  
 XZ= -5.1366 YZ= -1.6802 ZZ= 32.4666  
 Eigenvalues: 27.5017 28.4347 38.0077  
 77 H Isotropic = 30.0370 Anisotropy = 6.9756  
 XX= 30.2807 YX= -0.8927 ZX= 0.7090  
 XY= -0.3941 YY= 26.1515 ZY= -2.0592  
 XZ= 1.4024 YZ= -2.6841 ZZ= 33.6789  
 Eigenvalues: 25.4439 29.9797 34.6875  
 78 H Isotropic = 30.0908 Anisotropy = 7.1319  
 XX= 27.0290 YX= 0.2458 ZX= -0.7089  
 XY= -0.0009 YY= 31.4192 ZY= 3.8660  
 XZ= -0.8819 YZ= 2.5050 ZZ= 31.8243  
 Eigenvalues: 26.7582 28.6688 34.8454  
 79 H Isotropic = 30.5565 Anisotropy = 7.2718  
 XX= 31.7026 YX= -1.3976 ZX= 2.5433  
 XY= -1.7031 YY= 33.4184 ZY= -2.3687  
 XZ= 1.8690 YZ= -2.1329 ZZ= 26.5484  
 Eigenvalues: 25.3948 30.8703 35.4043  
 80 H Isotropic = 31.4078 Anisotropy = 10.4220  
 XX= 32.1707 YX= 4.5916 ZX= -1.4356  
 XY= 5.0500 YY= 34.0913 ZY= -1.0269  
 XZ= -1.4824 YZ= -1.2137 ZZ= 27.9615  
 Eigenvalues: 27.4357 28.4320 38.3558  
 81 H Isotropic = 28.1716 Anisotropy = 5.3165  
 XX= 30.7536 YX= 1.6127 ZX= -0.7903  
 XY= 1.3394 YY= 25.5417 ZY= 0.4964  
 XZ= -2.0087 YZ= -0.9831 ZZ= 28.2196

Eigenvalues: 25.1473 27.6517 31.7159  
82 H Isotropic = 31.8985 Anisotropy = 18.7028  
XX= 35.8162 YX= -3.6302 ZX= 8.1991  
XY= -3.7356 YY= 25.4811 ZY= 0.0027  
XZ= 9.3529 YZ= -0.6009 ZZ= 34.3980

Eigenvalues: 23.3269 28.0015 44.3670  
83 H Isotropic = 30.9623 Anisotropy = 10.4119  
XX= 34.7086 YX= -3.6047 ZX= 2.6713  
XY= -4.2248 YY= 30.3235 ZY= -1.6614  
XZ= 2.8742 YZ= -0.7679 ZZ= 27.8548

Eigenvalues: 26.8570 28.1263 37.9035  
84 H Isotropic = 30.4574 Anisotropy = 5.6298  
XX= 33.2391 YX= 0.1708 ZX= -0.7705  
XY= 1.3141 YY= 31.8145 ZY= -3.2128  
XZ= -1.0717 YZ= -2.5444 ZZ= 26.3186

Eigenvalues: 25.0487 32.1130 34.2106  
85 H Isotropic = 30.3468 Anisotropy = 7.6880  
XX= 28.3118 YX= -3.4543 ZX= -0.4992  
XY= -3.2587 YY= 30.9378 ZY= 3.6876  
XZ= -0.2037 YZ= 2.5705 ZZ= 31.7908

Eigenvalues: 25.6009 29.9674 35.4721  
86 O Isotropic = -90.9091 Anisotropy = 612.7933  
XX= -223.9538 YX= -116.4504 ZX= 47.2792  
XY= -118.8209 YY= 18.3363 ZY= -299.2360  
XZ= 35.2576 YZ= -329.2166 ZZ= -67.1099  
Eigenvalues: -360.0458 -230.3013 317.6198

## Conformer 6

1 C Isotropic = 13.5639 Anisotropy = 87.8459  
XX= -67.7108 YX= -9.4287 ZX= 49.8755  
XY= -26.9314 YY= 58.7909 ZY= 0.5215  
XZ= 27.7727 YZ= -13.1247 ZZ= 49.6115  
Eigenvalues: -81.1434 49.7072 72.1278

2 C Isotropic = 64.5305 Anisotropy = 104.0285  
XX= 84.4624 YX= 1.7887 ZX= -9.7984  
XY= 9.1153 YY= 51.7001 ZY= -82.1058  
XZ= -6.8273 YZ= -72.5610 ZZ= 57.4290  
Eigenvalues: -22.8537 82.5623 133.8828

3 C Isotropic = 22.9989 Anisotropy = 205.8732  
XX= 0.2426 YX= 37.8999 ZX= -17.9018  
XY= 26.5178 YY= 23.9190 ZY= -113.9320  
XZ= -20.8095 YZ= -120.6119 ZZ= 44.8352  
Eigenvalues: -84.7994 -6.4517 160.2477

4 C Isotropic = 46.6128 Anisotropy = 120.2842  
XX= 76.8892 YX= -2.3840 ZX= -43.7527  
XY= -2.1481 YY= 35.5525 ZY= -78.3955  
XZ= -45.6424 YZ= -72.7979 ZZ= 27.3968  
Eigenvalues: -53.4755 66.5116 126.8023

5 C Isotropic = 42.8697 Anisotropy = 183.0302  
XX= 65.1831 YX= 30.6113 ZX= -53.4762  
XY= 21.3677 YY= 16.0811 ZY= -93.6340  
XZ= -54.6306 YZ= -102.0914 ZZ= 47.3449  
Eigenvalues: -69.3792 33.0984 164.8898

6 C Isotropic = 137.1170 Anisotropy = 28.1659

XX= 117.1547 YX= -4.1255 ZX= -11.1539  
 XY= -1.6656 YY= 153.2322 ZY= -3.4914  
 XZ= -3.0353 YZ= -9.1166 ZZ= 140.9643  
 Eigenvalues: 114.6702 140.7866 155.8943  
 7 C Isotropic = 110.1550 Anisotropy = 49.6956  
 XX= 104.8758 YX= -14.3735 ZX= -14.5056  
 XY= -16.2908 YY= 128.5109 ZY= 12.6391  
 XZ= -14.9844 YZ= 13.0539 ZZ= 97.0781  
 Eigenvalues: 85.7023 101.4772 143.2854  
 8 C Isotropic = 139.4994 Anisotropy = 42.1342  
 XX= 153.8033 YX= -4.2532 ZX= -24.6301  
 XY= -2.6697 YY= 131.3586 ZY= 9.3250  
 XZ= -15.5326 YZ= 7.1843 ZZ= 133.3363  
 Eigenvalues: 118.6687 132.2406 167.5888  
 9 C Isotropic = 34.5984 Anisotropy = 178.4978  
 XX= -28.2701 YX= 78.6397 ZX= 11.4947  
 XY= 79.4137 YY= 79.5616 ZY= -65.9893  
 XZ= 7.7811 YZ= -68.7624 ZZ= 52.5036  
 Eigenvalues: -83.2489 33.4471 153.5969  
 10 C Isotropic = 47.9229 Anisotropy = 107.7053  
 XX= 43.5842 YX= 15.5962 ZX= -48.6584  
 XY= 14.3365 YY= 108.0372 ZY= 37.9290  
 XZ= -51.7869 YZ= 39.3026 ZZ= -7.8528  
 Eigenvalues: -49.1542 73.1964 119.7264  
 11 C Isotropic = 41.4562 Anisotropy = 176.0044  
 XX= -3.8246 YX= 34.9334 ZX= -41.5721  
 XY= 40.1008 YY= 140.4253 ZY= 46.6285  
 XZ= -28.0122 YZ= 49.1411 ZZ= -12.2319  
 Eigenvalues: -61.3588 26.9350 158.7925  
 12 C Isotropic = 135.7700 Anisotropy = 39.9432  
 XX= 150.8222 YX= -17.9486 ZX= 14.1798  
 XY= -16.4072 YY= 124.9243 ZY= -3.8076  
 XZ= 8.1397 YZ= 5.9023 ZZ= 131.5634  
 Eigenvalues: 114.0982 130.8130 162.3987  
 13 C Isotropic = 105.6923 Anisotropy = 79.7924  
 XX= 138.6022 YX= -11.0309 ZX= 37.6361  
 XY= -9.8632 YY= 92.6230 ZY= -11.5431  
 XZ= 34.2169 YZ= 0.6853 ZZ= 85.8517  
 Eigenvalues: 67.6576 90.5321 158.8873  
 14 C Isotropic = 150.0889 Anisotropy = 29.9184  
 XX= 147.7696 YX= -2.4395 ZX= 2.3051  
 XY= 5.2108 YY= 158.2003 ZY= -18.0694  
 XZ= 15.9406 YZ= -15.2191 ZZ= 144.2967  
 Eigenvalues: 129.3380 150.8942 170.0345  
 15 C Isotropic = 102.6836 Anisotropy = 32.1058  
 XX= 117.7909 YX= -1.9814 ZX= -16.1336  
 XY= -6.1651 YY= 78.7175 ZY= -4.1408  
 XZ= -1.6417 YZ= -7.2655 ZZ= 111.5426  
 Eigenvalues: 76.9798 106.9836 124.0875  
 16 C Isotropic = 95.1531 Anisotropy = 63.4939  
 XX= 80.5416 YX= 4.5669 ZX= 14.5256  
 XY= 4.0084 YY= 117.2767 ZY= -27.3038  
 XZ= 7.5600 YZ= -35.9516 ZZ= 87.6409  
 Eigenvalues: 60.7029 87.2740 137.4823  
 17 C Isotropic = 111.9831 Anisotropy = 42.6215

XX= 93.7922 YX= 2.2564 ZX= 3.5070  
 XY= 9.6038 YY= 121.9189 ZY= -15.7331  
 XZ= -0.7988 YZ= -22.3794 ZZ= 120.2382  
 Eigenvalues: 91.1806 104.3713 140.3974  
 18 C Isotropic = 54.1139 Anisotropy = 108.6449  
 XX= -22.8793 YX= 41.0649 ZX= -20.6887  
 XY= 45.3598 YY= 60.4245 ZY= -2.7231  
 XZ= -11.5607 YZ= 10.8079 ZZ= 124.7966  
 Eigenvalues: -42.8546 78.6525 126.5438  
 19 C Isotropic = 39.1108 Anisotropy = 176.6596  
 XX= -57.0733 YX= 35.7464 ZX= -27.0606  
 XY= 24.9879 YY= 22.1750 ZY= 0.2175  
 XZ= -35.8023 YZ= 4.3845 ZZ= 152.2306  
 Eigenvalues: -71.5413 31.9898 156.8839  
 20 C Isotropic = 139.7863 Anisotropy = 17.4693  
 XX= 148.1824 YX= 8.6865 ZX= -0.1245  
 XY= 3.3522 YY= 140.1681 ZY= 2.9442  
 XZ= 0.0243 YZ= 0.3260 ZZ= 131.0084  
 Eigenvalues: 130.6423 137.2841 151.4325  
 21 C Isotropic = 106.9813 Anisotropy = 32.0448  
 XX= 106.8679 YX= 0.5699 ZX= -6.7213  
 XY= -6.1646 YY= 125.5804 ZY= -9.1393  
 XZ= -6.4337 YZ= -11.6314 ZZ= 88.4956  
 Eigenvalues: 83.6315 108.9679 128.3445  
 22 C Isotropic = 142.9113 Anisotropy = 19.2196  
 XX= 148.6433 YX= -10.6966 ZX= -3.5679  
 XY= -4.5274 YY= 147.0141 ZY= 2.3581  
 XZ= -0.8309 YZ= -0.2791 ZZ= 133.0765  
 Eigenvalues: 132.7717 140.2378 155.7244  
 23 C Isotropic = 112.3857 Anisotropy = 47.1327  
 XX= 106.8256 YX= 9.6858 ZX= 11.9980  
 XY= 15.2766 YY= 125.4262 ZY= 18.8766  
 XZ= 11.0045 YZ= 18.1048 ZZ= 104.9052  
 Eigenvalues: 92.4400 100.9096 143.8074  
 24 C Isotropic = 166.0282 Anisotropy = 32.2670  
 XX= 186.8516 YX= 2.3936 ZX= -2.5625  
 XY= -5.4309 YY= 157.4556 ZY= 5.0497  
 XZ= -5.9815 YZ= 3.9079 ZZ= 153.7775  
 Eigenvalues: 150.5659 159.9793 187.5396  
 25 C Isotropic = 172.0158 Anisotropy = 15.7240  
 XX= 164.6577 YX= 12.3523 ZX= -0.9097  
 XY= 12.7546 YY= 173.3233 ZY= -0.3303  
 XZ= 4.1117 YZ= 0.4999 ZZ= 178.0665  
 Eigenvalues: 155.6401 177.9089 182.4985  
 26 C Isotropic = 69.3030 Anisotropy = 144.6886  
 XX= 13.6208 YX= 69.2920 ZX= 6.7803  
 XY= 66.3657 YY= 91.6385 ZY= -61.2038  
 XZ= 12.7072 YZ= -52.2166 ZZ= 102.6496  
 Eigenvalues: -36.2777 78.4246 165.7620  
 27 C Isotropic = 167.9356 Anisotropy = 26.9780  
 XX= 156.2570 YX= 0.5222 ZX= 2.1912  
 XY= 5.6333 YY= 173.8234 ZY= -14.8713  
 XZ= 5.4212 YZ= -9.4027 ZZ= 173.7265  
 Eigenvalues: 153.3790 164.5069 185.9210  
 28 C Isotropic = 165.8595 Anisotropy = 31.2003

XX= 174.5675 YX= -11.1735 ZX= -5.6224  
 XY= -10.7552 YY= 170.6468 ZY= 2.5236  
 XZ= -11.1279 YZ= 8.5939 ZZ= 152.3641  
 Eigenvalues: 149.3593 161.5594 186.6597  
 29 C Isotropic = 163.4276 Anisotropy = 20.4219  
 XX= 168.4629 YX= -9.6634 ZX= 0.2681  
 XY= -11.9181 YY= 160.9962 ZY= 4.4215  
 XZ= 0.3712 YZ= 9.0460 ZZ= 160.8236  
 Eigenvalues: 150.1479 163.0926 177.0422  
 30 C Isotropic = 169.7540 Anisotropy = 28.3555  
 XX= 168.7159 YX= 4.5913 ZX= -3.4638  
 XY= 8.0518 YY= 153.2524 ZY= -4.7295  
 XZ= -5.8662 YZ= 1.6513 ZZ= 187.2936  
 Eigenvalues: 150.9967 169.6077 188.6576  
 31 C Isotropic = 169.6528 Anisotropy = 30.8795  
 XX= 158.5875 YX= 10.2536 ZX= 5.2399  
 XY= 4.1243 YY= 167.0479 ZY= 12.7942  
 XZ= 1.0672 YZ= 9.6334 ZZ= 183.3231  
 Eigenvalues: 154.1081 164.6112 190.2392  
 32 O Isotropic = 100.6427 Anisotropy = 131.0602  
 XX= 164.7596 YX= 0.9068 ZX= 31.2095  
 XY= 77.9751 YY= 83.9618 ZY= -142.2388  
 XZ= 80.3809 YZ= -58.8942 ZZ= 53.2066  
 Eigenvalues: -54.2935 168.2053 188.0161  
 33 O Isotropic = 244.4969 Anisotropy = 35.0629  
 XX= 238.5515 YX= -5.2497 ZX= -3.2964  
 XY= -16.2691 YY= 261.9057 ZY= 3.1272  
 XZ= -6.3145 YZ= 9.9257 ZZ= 233.0334  
 Eigenvalues: 230.2475 235.3710 267.8722  
 34 O Isotropic = 220.2654 Anisotropy = 82.2068  
 XX= 241.0979 YX= 24.0798 ZX= 37.2327  
 XY= 30.9469 YY= 252.7868 ZY= -33.1347  
 XZ= 42.4351 YZ= -31.0420 ZZ= 166.9114  
 Eigenvalues: 135.5057 250.2205 275.0699  
 35 O Isotropic = 277.9004 Anisotropy = 73.5367  
 XX= 301.7312 YX= 37.5459 ZX= -6.6652  
 XY= 27.3792 YY= 280.9369 ZY= -22.9241  
 XZ= 6.5821 YZ= -12.5016 ZZ= 251.0330  
 Eigenvalues: 238.7420 268.0343 326.9248  
 36 O Isotropic = 268.2729 Anisotropy = 63.2841  
 XX= 215.0167 YX= 31.6964 ZX= -5.3337  
 XY= 5.9189 YY= 283.3254 ZY= 7.8336  
 XZ= 0.4583 YZ= 12.3032 ZZ= 306.4765  
 Eigenvalues: 209.9325 284.4239 310.4623  
 37 O Isotropic = 266.4862 Anisotropy = 60.1379  
 XX= 272.3382 YX= -13.6217 ZX= 3.4125  
 XY= 0.0547 YY= 305.0894 ZY= 13.4138  
 XZ= 7.9411 YZ= -4.2046 ZZ= 222.0311  
 Eigenvalues: 221.0577 271.8229 306.5781  
 38 H Isotropic = 25.8493 Anisotropy = 8.8501  
 XX= 30.7809 YX= -1.5071 ZX= -1.5709  
 XY= -2.4128 YY= 22.9696 ZY= -1.9912  
 XZ= -3.0995 YZ= -0.7736 ZZ= 23.7974  
 Eigenvalues: 21.0262 24.7723 31.7494  
 39 H Isotropic = 30.2177 Anisotropy = 8.8006

XX= 33.9430 YX= 2.2759 ZX= -2.4224  
 XY= 3.8993 YY= 30.3412 ZY= 0.6345  
 XZ= -2.2202 YZ= -0.0430 ZZ= 26.3689  
 Eigenvalues: 25.4013 29.1670 36.0848  
 40 H Isotropic = 30.1707 Anisotropy = 6.1629  
 XX= 28.2219 YX= -0.0949 ZX= 0.7596  
 XY= -0.5211 YY= 29.9886 ZY= -2.7716  
 XZ= 2.4611 YZ= -2.2124 ZZ= 32.3015  
 Eigenvalues: 27.4658 28.7669 34.2793  
 41 H Isotropic = 27.8866 Anisotropy = 8.1417  
 XX= 30.8056 YX= -0.9534 ZX= 0.0585  
 XY= -3.0145 YY= 30.7127 ZY= 3.1490  
 XZ= -0.7843 YZ= 3.0550 ZZ= 22.1415  
 Eigenvalues: 21.1290 29.2164 33.3144  
 42 H Isotropic = 25.2513 Anisotropy = 6.3991  
 XX= 27.4059 YX= -3.0122 ZX= -1.5398  
 XY= -3.3466 YY= 24.6817 ZY= -2.5502  
 XZ= -1.8217 YZ= -1.5783 ZZ= 23.6663  
 Eigenvalues: 20.4193 25.8173 29.5174  
 43 H Isotropic = 25.4193 Anisotropy = 7.2093  
 XX= 26.6558 YX= -1.8715 ZX= -1.7996  
 XY= -3.0441 YY= 28.4987 ZY= -1.4806  
 XZ= -2.5687 YZ= -0.4906 ZZ= 21.1033  
 Eigenvalues: 19.9702 26.0621 30.2254  
 44 H Isotropic = 30.0443 Anisotropy = 3.6914  
 XX= 28.7552 YX= -2.3472 ZX= -0.9537  
 XY= -1.0896 YY= 28.9954 ZY= 0.5195  
 XZ= 0.6198 YZ= 0.4490 ZZ= 32.3823  
 Eigenvalues: 27.1443 30.4834 32.5052  
 45 H Isotropic = 28.6634 Anisotropy = 7.1386  
 XX= 32.1433 YX= 0.1827 ZX= -2.2437  
 XY= 1.0109 YY= 27.4344 ZY= -1.0642  
 XZ= -3.4707 YZ= -0.0573 ZZ= 26.4124  
 Eigenvalues: 25.1925 27.3752 33.4225  
 46 H Isotropic = 27.8264 Anisotropy = 3.1288  
 XX= 27.8957 YX= -1.7144 ZX= 0.5219  
 XY= -1.3868 YY= 26.7673 ZY= 2.3457  
 XZ= 1.3190 YZ= 1.3674 ZZ= 28.8163  
 Eigenvalues: 24.6649 28.9021 29.9123  
 47 H Isotropic = 31.5709 Anisotropy = 13.3191  
 XX= 28.7131 YX= -0.7916 ZX= 3.1394  
 XY= -0.6499 YY= 32.2317 ZY= 7.3450  
 XZ= 3.1999 YZ= 6.8469 ZZ= 33.7677  
 Eigenvalues: 24.2156 30.0467 40.4503  
 48 H Isotropic = 30.2581 Anisotropy = 4.1738  
 XX= 32.9185 YX= -0.4699 ZX= 0.0520  
 XY= -0.9471 YY= 28.8914 ZY= 2.0249  
 XZ= 0.1135 YZ= -0.2719 ZZ= 28.9645  
 Eigenvalues: 27.9838 29.7500 33.0406  
 49 H Isotropic = 29.0834 Anisotropy = 5.4402  
 XX= 27.2469 YX= 0.8482 ZX= -2.2653  
 XY= -1.8176 YY= 32.4760 ZY= -0.7304  
 XZ= -2.3323 YZ= -1.4729 ZZ= 27.5273  
 Eigenvalues: 24.9205 29.6195 32.7102  
 50 H Isotropic = 26.7311 Anisotropy = 5.2788

XX= 27.8725 YX= 2.7501 ZX= 3.3780  
 XY= 1.7836 YY= 25.1513 ZY= -0.1876  
 XZ= 0.8920 YZ= -0.1851 ZZ= 27.1694  
 Eigenvalues: 23.4099 26.5330 30.2503  
 51 H Isotropic = 26.5777 Anisotropy = 6.1047  
 XX= 24.9502 YX= 0.0107 ZX= -0.4176  
 XY= 1.4818 YY= 24.5780 ZY= 1.3980  
 XZ= 3.0880 YZ= 0.0117 ZZ= 30.2051  
 Eigenvalues: 23.9802 25.1055 30.6475  
 52 H Isotropic = 26.0695 Anisotropy = 9.1111  
 XX= 30.6802 YX= -0.8923 ZX= -4.1124  
 XY= -1.4499 YY= 25.8756 ZY= 0.1893  
 XZ= -3.1972 YZ= -0.6487 ZZ= 21.6526  
 Eigenvalues: 20.2913 25.7736 32.1435  
 53 H Isotropic = 30.4440 Anisotropy = 5.7530  
 XX= 28.1979 YX= -1.4198 ZX= 1.4186  
 XY= -1.4245 YY= 30.1299 ZY= 2.3488  
 XZ= 0.7578 YZ= 2.2215 ZZ= 33.0042  
 Eigenvalues: 26.7248 30.3279 34.2793  
 54 H Isotropic = 29.4475 Anisotropy = 6.7060  
 XX= 32.5454 YX= -2.2965 ZX= -0.7853  
 XY= -2.9706 YY= 27.1651 ZY= -2.9157  
 XZ= 0.7783 YZ= -3.0945 ZZ= 28.6318  
 Eigenvalues: 24.2605 30.1637 33.9182  
 55 H Isotropic = 30.4083 Anisotropy = 8.0881  
 XX= 31.6354 YX= 1.2867 ZX= -0.4332  
 XY= 3.5003 YY= 30.5129 ZY= -4.9145  
 XZ= -1.5049 YZ= -4.0556 ZZ= 29.0767  
 Eigenvalues: 25.1388 30.2858 35.8004  
 56 H Isotropic = 28.9937 Anisotropy = 4.7538  
 XX= 30.7403 YX= -2.6448 ZX= 0.3969  
 XY= -1.8998 YY= 28.5040 ZY= -0.6641  
 XZ= -1.0102 YZ= -1.0310 ZZ= 27.7369  
 Eigenvalues: 26.4721 28.3462 32.1629  
 57 H Isotropic = 28.9810 Anisotropy = 5.2589  
 XX= 31.2294 YX= 0.0755 ZX= 1.0504  
 XY= 1.6517 YY= 30.5840 ZY= 1.0752  
 XZ= 2.8386 YZ= 1.0285 ZZ= 25.1295  
 Eigenvalues: 24.4632 29.9928 32.4869  
 58 H Isotropic = 27.2927 Anisotropy = 6.6826  
 XX= 27.5825 YX= -2.1860 ZX= 1.5001  
 XY= -1.5568 YY= 25.4842 ZY= -3.0938  
 XZ= 0.1765 YZ= -3.9010 ZZ= 28.8116  
 Eigenvalues: 22.9720 27.1584 31.7478  
 59 H Isotropic = 30.0232 Anisotropy = 6.2167  
 XX= 33.6777 YX= 0.7408 ZX= 1.6143  
 XY= 0.4233 YY= 28.8774 ZY= -1.3078  
 XZ= 1.9052 YZ= -0.3987 ZZ= 27.5143  
 Eigenvalues: 26.6234 29.2784 34.1676  
 60 H Isotropic = 29.6298 Anisotropy = 9.1527  
 XX= 26.7350 YX= -0.8984 ZX= -0.8148  
 XY= -0.5752 YY= 27.7384 ZY= 2.8241  
 XZ= 0.1163 YZ= 3.5466 ZZ= 34.4159  
 Eigenvalues: 26.0138 27.1439 35.7315  
 61 H Isotropic = 26.6094 Anisotropy = 3.3285

XX= 28.2609 YX= -0.8471 ZX= -1.5478  
 XY= 1.0046 YY= 28.3679 ZY= 0.4837  
 XZ= -1.7408 YZ= 1.2199 ZZ= 23.1995  
 Eigenvalues: 22.5903 28.4095 28.8285  
 62 H Isotropic = 30.4594 Anisotropy = 10.1128  
 XX= 36.4535 YX= 2.9468 ZX= -0.5632  
 XY= 2.3512 YY= 27.5684 ZY= 2.2924  
 XZ= -1.5798 YZ= 2.4227 ZZ= 27.3564  
 Eigenvalues: 24.5210 29.6559 37.2013  
 63 H Isotropic = 31.1998 Anisotropy = 7.2078  
 XX= 31.5352 YX= -1.6283 ZX= -0.4070  
 XY= -1.3269 YY= 28.6500 ZY= 4.2835  
 XZ= -0.1376 YZ= 3.9450 ZZ= 33.4142  
 Eigenvalues: 26.0357 31.5587 36.0050  
 64 H Isotropic = 30.2467 Anisotropy = 8.7468  
 XX= 29.1190 YX= -3.7431 ZX= 0.4036  
 XY= -3.4678 YY= 34.1403 ZY= -1.4296  
 XZ= -0.1676 YZ= 0.0047 ZZ= 27.4808  
 Eigenvalues: 27.0873 27.5748 36.0779  
 65 H Isotropic = 26.7791 Anisotropy = 2.4203  
 XX= 27.3885 YX= 0.3471 ZX= 0.7541  
 XY= 0.5970 YY= 28.1228 ZY= 0.4376  
 XZ= 0.0901 YZ= -0.0287 ZZ= 24.8261  
 Eigenvalues: 24.7534 27.1913 28.3926  
 66 H Isotropic = 30.4774 Anisotropy = 17.0317  
 XX= 40.3367 YX= 3.9688 ZX= 0.1769  
 XY= 5.2887 YY= 25.9353 ZY= -5.7231  
 XZ= 0.1111 YZ= -5.3882 ZZ= 25.1602  
 Eigenvalues: 19.4455 30.1548 41.8319  
 67 H Isotropic = 26.0804 Anisotropy = 8.2545  
 XX= 28.0991 YX= 5.1790 ZX= 1.0372  
 XY= 3.4293 YY= 26.0340 ZY= 0.0119  
 XZ= 0.9796 YZ= 0.0805 ZZ= 24.1080  
 Eigenvalues: 22.4253 24.2325 31.5833  
 68 H Isotropic = 29.4983 Anisotropy = 8.3577  
 XX= 34.5325 YX= 2.6887 ZX= 1.0166  
 XY= 0.4728 YY= 28.8624 ZY= 2.2649  
 XZ= 0.2732 YZ= 1.5163 ZZ= 25.0999  
 Eigenvalues: 24.3141 29.1107 35.0701  
 69 H Isotropic = 30.5209 Anisotropy = 7.3672  
 XX= 30.9888 YX= -0.5273 ZX= -0.3907  
 XY= 0.7946 YY= 31.2987 ZY= 4.7482  
 XZ= 0.0025 YZ= 5.3415 ZZ= 29.2754  
 Eigenvalues: 25.1323 30.9981 35.4324  
 70 H Isotropic = 29.2783 Anisotropy = 3.3606  
 XX= 30.9366 YX= 1.2472 ZX= 1.2205  
 XY= 1.3677 YY= 28.1953 ZY= -2.4857  
 XZ= 0.9846 YZ= -3.5279 ZZ= 28.7029  
 Eigenvalues: 24.9443 31.3718 31.5187  
 71 H Isotropic = 30.2182 Anisotropy = 4.2797  
 XX= 32.2829 YX= 2.1609 ZX= -0.0692  
 XY= 1.1999 YY= 27.0890 ZY= 1.5875  
 XZ= 0.0442 YZ= 2.6102 ZZ= 31.2827  
 Eigenvalues: 25.8390 31.7442 33.0713  
 72 H Isotropic = 28.9364 Anisotropy = 5.4910

XX= 32.1037 YX= -0.4396 ZX= -1.1427  
 XY= 1.1600 YY= 28.8691 ZY= -3.1645  
 XZ= -1.1029 YZ= -2.8306 ZZ= 25.8363  
 Eigenvalues: 23.9203 30.2918 32.5971  
 73 H Isotropic = 27.9963 Anisotropy = 4.9525  
 XX= 31.2058 YX= 0.1713 ZX= 0.1940  
 XY= 0.7898 YY= 28.3594 ZY= 2.4145  
 XZ= -0.1697 YZ= 0.9104 ZZ= 24.4237  
 Eigenvalues: 23.8122 28.8787 31.2980  
 74 H Isotropic = 32.2224 Anisotropy = 13.4969  
 XX= 29.3999 YX= -1.7456 ZX= 1.4446  
 XY= -0.8266 YY= 35.1656 ZY= 7.2725  
 XZ= 0.3830 YZ= 7.5574 ZZ= 32.1017  
 Eigenvalues: 25.4717 29.9752 41.2203  
 75 H Isotropic = 30.6794 Anisotropy = 8.3035  
 XX= 27.4774 YX= 0.8234 ZX= -0.1115  
 XY= 0.7232 YY= 28.8716 ZY= 1.3483  
 XZ= 0.0003 YZ= 2.5724 ZZ= 35.6890  
 Eigenvalues: 27.0339 28.7892 36.2150  
 76 H Isotropic = 31.4460 Anisotropy = 9.5156  
 XX= 35.7139 YX= 1.4681 ZX= -2.8155  
 XY= 2.2476 YY= 28.9823 ZY= -2.1901  
 XZ= -3.5321 YZ= -1.8329 ZZ= 29.6418  
 Eigenvalues: 27.1975 29.3507 37.7897  
 77 H Isotropic = 30.1845 Anisotropy = 7.0551  
 XX= 29.5496 YX= -2.1514 ZX= -1.6512  
 XY= -1.8132 YY= 31.6067 ZY= -4.0104  
 XZ= -1.4445 YZ= -4.3036 ZZ= 29.3972  
 Eigenvalues: 24.9109 30.7547 34.8879  
 78 H Isotropic = 31.1766 Anisotropy = 8.4536  
 XX= 29.8964 YX= 1.6795 ZX= 0.5592  
 XY= 1.2934 YY= 26.9244 ZY= 1.6359  
 XZ= -0.4259 YZ= 0.3187 ZZ= 36.7089  
 Eigenvalues: 26.2348 30.4826 36.8123  
 79 H Isotropic = 31.0146 Anisotropy = 8.2028  
 XX= 29.7714 YX= 0.7893 ZX= 1.3594  
 XY= -0.1618 YY= 35.8533 ZY= 2.0244  
 XZ= 1.0868 YZ= 2.5256 ZZ= 27.4192  
 Eigenvalues: 26.4682 30.0926 36.4831  
 80 H Isotropic = 31.2335 Anisotropy = 9.2590  
 XX= 36.2635 YX= 1.7093 ZX= 1.7075  
 XY= 2.1432 YY= 29.3190 ZY= 2.2982  
 XZ= 2.0711 YZ= 2.2562 ZZ= 28.1180  
 Eigenvalues: 26.3511 29.9432 37.4062  
 81 H Isotropic = 27.9239 Anisotropy = 1.4583  
 XX= 28.4397 YX= 0.0028 ZX= 0.6884  
 XY= -0.1256 YY= 26.6191 ZY= -0.1865  
 XZ= -0.7778 YZ= -1.0995 ZZ= 28.7129  
 Eigenvalues: 26.4349 28.4407 28.8961  
 82 H Isotropic = 31.8977 Anisotropy = 17.5039  
 XX= 29.2397 YX= -2.6301 ZX= 1.8722  
 XY= -3.0590 YY= 42.8987 ZY= 1.3559  
 XZ= 1.4873 YZ= 2.1766 ZZ= 23.5548  
 Eigenvalues: 22.7846 29.3415 43.5670  
 83 H Isotropic = 30.9435 Anisotropy = 9.9100

XX= 32.0636 YX= -4.7215 ZX= 0.8487  
XY= -3.8044 YY= 33.5881 ZY= -2.1143  
XZ= 0.9490 YZ= -1.6442 ZZ= 27.1788  
Eigenvalues: 26.6468 28.6335 37.5502

84 H Isotropic = 30.5449 Anisotropy = 6.8616  
XX= 31.2542 YX= -2.1022 ZX= -3.9054  
XY= -2.2550 YY= 28.5404 ZY= -0.2768  
XZ= -2.7955 YZ= -0.6677 ZZ= 31.8400  
Eigenvalues: 26.3602 30.1551 35.1193

85 H Isotropic = 30.5622 Anisotropy = 9.5177  
XX= 35.5125 YX= 1.2739 ZX= 3.5674  
XY= 0.4135 YY= 29.4843 ZY= 2.3205  
XZ= 2.9702 YZ= 2.1343 ZZ= 26.6899  
Eigenvalues: 24.8414 29.9378 36.9074

86 O Isotropic = -90.8674 Anisotropy = 614.0413  
XX= -208.6237 YX= -132.2380 ZX= 83.3055  
XY= -135.4814 YY= -69.1702 ZY= -290.4248  
XZ= 71.7803 YZ= -323.7089 ZZ= 5.1918  
Eigenvalues: -361.2857 -229.8099 318.4935

## Conformer 7

1 C Isotropic = 13.5283 Anisotropy = 87.4686  
XX= -45.2194 YX= 21.5937 ZX= -70.0454  
XY= -0.3299 YY= 52.0053 ZY= 6.5816  
XZ= -55.0097 YZ= 23.4960 ZZ= 33.7989  
Eigenvalues: -81.7338 50.4779 71.8406

2 C Isotropic = 64.9415 Anisotropy = 103.3271  
XX= 78.8803 YX= -22.0675 ZX= 9.9119  
XY= -16.9241 YY= -2.0025 ZY= 51.5256  
XZ= 9.2016 YZ= 40.8781 ZZ= 117.9466  
Eigenvalues: -22.3201 83.3183 133.8262

3 C Isotropic = 22.6965 Anisotropy = 206.7663  
XX= -6.5430 YX= 5.0842 ZX= 13.6327  
XY= -4.9002 YY= -63.0071 ZY= 65.6902  
XZ= 12.6255 YZ= 74.1363 ZZ= 137.6395  
Eigenvalues: -85.1545 -7.2968 160.5407

4 C Isotropic = 46.0370 Anisotropy = 120.7871  
XX= 52.8040 YX= -39.3733 ZX= 40.2322  
XY= -40.5782 YY= -15.4516 ZY= 45.0720  
XZ= 40.7912 YZ= 40.1924 ZZ= 100.7585  
Eigenvalues: -54.2598 65.8090 126.5617

5 C Isotropic = 41.6727 Anisotropy = 185.4364  
XX= 37.6463 YX= -17.8683 ZX= 54.2983  
XY= -25.8473 YY= -49.3147 ZY= 39.9110  
XZ= 52.8040 YZ= 50.4232 ZZ= 136.6864  
Eigenvalues: -70.9784 30.6994 165.2970

6 C Isotropic = 141.2832 Anisotropy = 21.7166  
XX= 121.9819 YX= -5.1892 ZX= 3.5168  
XY= -0.0205 YY= 150.3845 ZY= 3.9983  
XZ= -1.6519 YZ= 5.5275 ZZ= 151.4833  
Eigenvalues: 121.6813 146.4075 155.7609

7 C Isotropic = 109.9710 Anisotropy = 48.0492  
XX= 100.7537 YX= -12.8756 ZX= 7.6796  
XY= -13.7084 YY= 136.9851 ZY= -4.1525

XZ= 7.1210 YZ= -3.0248 ZZ= 92.1742  
 Eigenvalues: 87.5931 100.3160 142.0038  
 8 C Isotropic = 138.6451 Anisotropy = 40.4293  
 XX= 140.4703 YX= -14.3883 ZX= 22.6040  
 XY= -9.1976 YY= 141.3611 ZY= -8.9722  
 XZ= 15.5837 YZ= -8.7517 ZZ= 134.1039  
 Eigenvalues: 117.8883 132.4490 165.5979  
 9 C Isotropic = 34.3974 Anisotropy = 179.3883  
 XX= -14.9847 YX= 69.7873 ZX= 4.0679  
 XY= 68.9679 YY= 6.0094 ZY= 67.3933  
 XZ= 7.7711 YZ= 68.7815 ZZ= 112.1675  
 Eigenvalues: -83.7406 32.9432 153.9896  
 10 C Isotropic = 47.5636 Anisotropy = 109.2297  
 XX= 19.6477 YX= 4.7604 ZX= 59.9184  
 XY= 1.8443 YY= 118.8269 ZY= 9.3385  
 XZ= 62.2899 YZ= 8.0620 ZZ= 4.2161  
 Eigenvalues: -49.7697 72.0770 120.3834  
 11 C Isotropic = 42.2840 Anisotropy = 174.6076  
 XX= -14.4702 YX= 31.6248 ZX= 55.6882  
 XY= 41.3756 YY= 143.7748 ZY= 22.9716  
 XZ= 45.2151 YZ= 20.7937 ZZ= -2.4526  
 Eigenvalues: -60.1369 28.2998 158.6891  
 12 C Isotropic = 135.6048 Anisotropy = 39.6051  
 XX= 153.4505 YX= -11.8903 ZX= -15.1143  
 XY= -14.5539 YY= 129.7112 ZY= 1.6560  
 XZ= -9.7118 YZ= -8.9311 ZZ= 123.6528  
 Eigenvalues: 114.1989 130.6074 162.0082  
 13 C Isotropic = 105.4464 Anisotropy = 79.6135  
 XX= 150.9655 YX= -2.4226 ZX= -24.5601  
 XY= -5.5255 YY= 87.0457 ZY= 16.6921  
 XZ= -22.3541 YZ= 3.8903 ZZ= 78.3280  
 Eigenvalues: 67.4127 90.4044 158.5221  
 14 C Isotropic = 150.0926 Anisotropy = 30.2989  
 XX= 151.4985 YX= -5.4598 ZX= -2.4566  
 XY= 6.4370 YY= 142.7581 ZY= 20.0053  
 XZ= -12.3985 YZ= 15.7053 ZZ= 156.0213  
 Eigenvalues: 129.3313 150.6548 170.2919  
 15 C Isotropic = 103.0412 Anisotropy = 31.6880  
 XX= 113.1375 YX= -10.9246 ZX= 13.0367  
 XY= -8.2382 YY= 82.5347 ZY= -13.1064  
 XZ= -1.2697 YZ= -8.4428 ZZ= 113.4513  
 Eigenvalues: 77.5382 107.4188 124.1665  
 16 C Isotropic = 95.4410 Anisotropy = 63.7100  
 XX= 86.1022 YX= 2.6304 ZX= -14.7052  
 XY= 0.8982 YY= 87.9533 ZY= 30.4316  
 XZ= -7.3895 YZ= 38.5047 ZZ= 112.2675  
 Eigenvalues: 61.0352 87.3734 137.9143  
 17 C Isotropic = 112.3997 Anisotropy = 42.2454  
 XX= 96.3602 YX= 2.1228 ZX= -9.4154  
 XY= 7.7094 YY= 106.6306 ZY= 11.9480  
 XZ= -2.9858 YZ= 16.4959 ZZ= 134.2084  
 Eigenvalues: 91.0327 105.6032 140.5633  
 18 C Isotropic = 52.3559 Anisotropy = 115.2445  
 XX= -20.8160 YX= 53.2788 ZX= 2.7090  
 XY= 51.1042 YY= 52.8372 ZY= -17.4947

XZ= 8.0006 YZ= -16.5453 ZZ= 125.0464  
 Eigenvalues: -48.7833 76.6654 129.1855  
 19 C Isotropic = 40.7335 Anisotropy = 174.1570  
 XX= -55.1267 YX= 38.0675 ZX= -8.6964  
 XY= 29.6698 YY= 41.8293 ZY= -46.4875  
 XZ= -4.4730 YZ= -47.6665 ZZ= 135.4979  
 Eigenvalues: -66.1226 31.4849 156.8382  
 20 C Isotropic = 142.7030 Anisotropy = 23.2569  
 XX= 158.2038 YX= -2.6740 ZX= -2.8649  
 XY= 2.9774 YY= 135.1037 ZY= 0.6985  
 XZ= 3.4115 YZ= -5.4331 ZZ= 134.8016  
 Eigenvalues: 132.5770 137.3245 158.2076  
 21 C Isotropic = 108.8568 Anisotropy = 33.4939  
 XX= 108.4477 YX= 9.6629 ZX= 9.5590  
 XY= 2.4593 YY= 109.6297 ZY= 19.5995  
 XZ= 1.3019 YZ= 18.8167 ZZ= 108.4932  
 Eigenvalues: 89.8386 105.5458 131.1861  
 22 C Isotropic = 144.0037 Anisotropy = 12.3437  
 XX= 152.1782 YX= 4.2200 ZX= -1.3047  
 XY= -2.7758 YY= 141.5482 ZY= -1.2513  
 XZ= 1.8209 YZ= 2.0706 ZZ= 138.2848  
 Eigenvalues: 138.2321 141.5462 152.2329  
 23 C Isotropic = 112.4310 Anisotropy = 40.5182  
 XX= 134.5305 YX= 5.8149 ZX= 4.8138  
 XY= 15.2963 YY= 107.3372 ZY= 5.0041  
 XZ= 7.5595 YZ= 5.3660 ZZ= 95.4253  
 Eigenvalues: 93.3478 104.5021 139.4432  
 24 C Isotropic = 164.2255 Anisotropy = 26.8166  
 XX= 163.6300 YX= -7.3029 ZX= 0.0710  
 XY= 0.9178 YY= 170.9200 ZY= 17.0040  
 XZ= 5.9803 YZ= 15.6418 ZZ= 158.1266  
 Eigenvalues: 145.9455 164.6279 182.1033  
 25 C Isotropic = 172.1180 Anisotropy = 15.5315  
 XX= 166.8988 YX= 12.1856 ZX= 3.2080  
 XY= 14.2675 YY= 170.8577 ZY= 0.7512  
 XZ= -1.0664 YZ= -0.1617 ZZ= 178.5976  
 Eigenvalues: 155.4879 178.3939 182.4724  
 26 C Isotropic = 69.0568 Anisotropy = 144.3895  
 XX= 27.3220 YX= 63.3268 ZX= 3.5734  
 XY= 60.7091 YY= 35.1526 ZY= 48.8412  
 XZ= -4.0422 YZ= 43.2231 ZZ= 144.6960  
 Eigenvalues: -36.7105 78.5645 165.3165  
 27 C Isotropic = 167.8701 Anisotropy = 27.0392  
 XX= 158.7748 YX= 1.0168 ZX= -5.0572  
 XY= 5.8623 YY= 163.7573 ZY= 12.5506  
 XZ= -6.7382 YZ= 6.4646 ZZ= 181.0781  
 Eigenvalues: 153.3481 164.3659 185.8962  
 28 C Isotropic = 165.9519 Anisotropy = 31.2241  
 XX= 168.3944 YX= -11.8329 ZX= 5.0653  
 XY= -15.2444 YY= 175.6021 ZY= 2.5491  
 XZ= 9.1054 YZ= -4.0918 ZZ= 153.8591  
 Eigenvalues: 149.9070 161.1806 186.7679  
 29 C Isotropic = 166.7657 Anisotropy = 19.0499  
 XX= 170.4287 YX= -7.3192 ZX= -1.9547  
 XY= -12.9358 YY= 167.5534 ZY= 2.7301

XZ= -3.8480 YZ= -3.1927 ZZ= 162.3150  
 Eigenvalues: 157.7707 163.0607 179.4656  
 30 C Isotropic = 160.1287 Anisotropy = 39.1787  
 XX= 143.1748 YX= -4.4005 ZX= -3.4077  
 XY= -8.0618 YY= 166.9527 ZY= 18.3469  
 XZ= -1.6096 YZ= 15.0689 ZZ= 170.2586  
 Eigenvalues: 141.5079 152.6304 186.2478  
 31 C Isotropic = 169.2880 Anisotropy = 25.8159  
 XX= 165.5942 YX= 1.8687 ZX= -7.8600  
 XY= 3.7618 YY= 163.7962 ZY= -11.3013  
 XZ= -10.1891 YZ= -5.4693 ZZ= 178.4737  
 Eigenvalues: 159.4105 161.9549 186.4986  
 32 O Isotropic = 103.0795 Anisotropy = 130.9149  
 XX= 187.8292 YX= -16.1421 ZX= -0.4601  
 XY= 54.9824 YY= -2.9566 ZY= 137.5928  
 XZ= -24.9924 YZ= 39.7322 ZZ= 124.3660  
 Eigenvalues: -50.6808 169.5633 190.3561  
 33 O Isotropic = 255.6562 Anisotropy = 92.9591  
 XX= 226.8210 YX= -30.6481 ZX= 21.1445  
 XY= -35.4678 YY= 262.7427 ZY= 36.4578  
 XZ= 2.8283 YZ= 53.6541 ZZ= 277.4049  
 Eigenvalues: 192.0597 257.2800 317.6289  
 34 O Isotropic = 219.9718 Anisotropy = 81.7710  
 XX= 255.4271 YX= 20.4989 ZX= -7.1657  
 XY= 27.9601 YY= 206.6034 ZY= 64.7771  
 XZ= -9.9490 YZ= 60.8622 ZZ= 197.8848  
 Eigenvalues: 134.9256 250.5040 274.4858  
 35 O Isotropic = 278.4001 Anisotropy = 73.1407  
 XX= 300.5025 YX= 22.8099 ZX= 30.9951  
 XY= 16.4742 YY= 257.2287 ZY= 28.6774  
 XZ= 13.4230 YZ= 21.7743 ZZ= 277.4691  
 Eigenvalues: 239.8419 268.1979 327.1606  
 36 O Isotropic = 270.5888 Anisotropy = 32.8825  
 XX= 289.6532 YX= -0.6299 ZX= -22.2599  
 XY= 7.7054 YY= 286.0469 ZY= 24.6187  
 XZ= 0.5166 YZ= -8.9055 ZZ= 236.0661  
 Eigenvalues: 232.6256 286.6302 292.5104  
 37 O Isotropic = 259.8828 Anisotropy = 62.9866  
 XX= 275.2719 YX= -10.5073 ZX= 32.3219  
 XY= -31.6108 YY= 279.4233 ZY= 6.8450  
 XZ= 32.6715 YZ= 15.2717 ZZ= 224.9532  
 Eigenvalues: 203.9768 273.7977 301.8738  
 38 H Isotropic = 25.8243 Anisotropy = 8.7713  
 XX= 29.2242 YX= -2.8057 ZX= 1.8249  
 XY= -4.4851 YY= 22.9003 ZY= 0.2173  
 XZ= 2.7638 YZ= -0.8522 ZZ= 25.3483  
 Eigenvalues: 21.1184 24.6827 31.6718  
 39 H Isotropic = 30.1826 Anisotropy = 8.7097  
 XX= 32.7103 YX= 0.2967 ZX= 4.3430  
 XY= 1.9246 YY= 29.4903 ZY= 0.9142  
 XZ= 4.9060 YZ= 1.1881 ZZ= 28.3473  
 Eigenvalues: 25.3934 29.1654 35.9891  
 40 H Isotropic = 30.2025 Anisotropy = 6.1906  
 XX= 29.1253 YX= 0.0888 ZX= -1.5492  
 XY= 0.2550 YY= 28.4702 ZY= 1.2913

XZ= -3.3489 YZ= 0.8372 ZZ= 33.0119  
 Eigenvalues: 27.4969 28.7810 34.3296  
 41 H Isotropic = 27.9082 Anisotropy = 8.0767  
 XX= 30.0873 YX= -0.7987 ZX= 1.4019  
 XY= -3.0149 YY= 32.1574 ZY= 0.4631  
 XZ= 1.3174 YZ= 0.9536 ZZ= 21.4798  
 Eigenvalues: 21.1779 29.2540 33.2926  
 42 H Isotropic = 25.2024 Anisotropy = 6.4236  
 XX= 26.2343 YX= -3.9122 ZX= 0.5590  
 XY= -4.5716 YY= 23.9491 ZY= 1.2202  
 XZ= 0.7023 YZ= 0.3568 ZZ= 25.4240  
 Eigenvalues: 20.4920 25.6305 29.4849  
 43 H Isotropic = 25.3502 Anisotropy = 7.2992  
 XX= 25.0465 YX= -2.7790 ZX= 1.8484  
 XY= -4.4009 YY= 27.4613 ZY= 3.0089  
 XZ= 1.9150 YZ= 2.1106 ZZ= 23.5428  
 Eigenvalues: 19.8957 25.9386 30.2163  
 44 H Isotropic = 29.6906 Anisotropy = 3.9803  
 XX= 28.7000 YX= -1.5608 ZX= -1.1496  
 XY= 0.1772 YY= 29.8453 ZY= -1.9147  
 XZ= -2.1630 YZ= -1.8896 ZZ= 30.5265  
 Eigenvalues: 26.8110 29.9167 32.3441  
 45 H Isotropic = 28.7384 Anisotropy = 7.7213  
 XX= 30.7177 YX= -1.4600 ZX= 3.2417  
 XY= -1.5121 YY= 26.9627 ZY= 0.7517  
 XZ= 4.6585 YZ= -0.3043 ZZ= 28.5348  
 Eigenvalues: 24.9217 27.4076 33.8859  
 46 H Isotropic = 27.5506 Anisotropy = 3.7612  
 XX= 28.0347 YX= -1.1318 ZX= -1.5443  
 XY= 0.1445 YY= 28.9294 ZY= -2.5600  
 XZ= -1.6657 YZ= -1.7576 ZZ= 25.6878  
 Eigenvalues: 23.9374 28.6563 30.0581  
 47 H Isotropic = 31.5005 Anisotropy = 16.6748  
 XX= 25.0992 YX= -4.3123 ZX= -2.2217  
 XY= -5.0169 YY= 33.9343 ZY= 7.4070  
 XZ= -2.5940 YZ= 5.5559 ZZ= 35.4680  
 Eigenvalues: 23.0783 28.8062 42.6171  
 48 H Isotropic = 29.8261 Anisotropy = 3.9873  
 XX= 32.2876 YX= -0.6902 ZX= 0.3468  
 XY= -0.7601 YY= 29.2260 ZY= -1.7944  
 XZ= 0.1373 YZ= 0.4395 ZZ= 27.9645  
 Eigenvalues: 27.6686 29.3253 32.4842  
 49 H Isotropic = 29.5993 Anisotropy = 5.3544  
 XX= 26.7453 YX= -0.1145 ZX= 2.0286  
 XY= -2.6081 YY= 31.7443 ZY= 1.3846  
 XZ= 1.2693 YZ= 2.6424 ZZ= 30.3082  
 Eigenvalues: 25.4282 30.2008 33.1688  
 50 H Isotropic = 26.7497 Anisotropy = 5.4170  
 XX= 29.0503 YX= 3.4737 ZX= -1.8240  
 XY= 1.6508 YY= 24.5951 ZY= -0.0592  
 XZ= 0.2120 YZ= 0.0672 ZZ= 26.6037  
 Eigenvalues: 23.3910 26.4969 30.3610  
 51 H Isotropic = 26.5586 Anisotropy = 6.2710  
 XX= 25.9132 YX= 0.2624 ZX= -0.6877  
 XY= 3.1908 YY= 25.4568 ZY= -2.6029

XZ= -3.1985 YZ= -1.5573 ZZ= 28.3059  
 Eigenvalues: 23.9055 25.0310 30.7393  
 52 H Isotropic = 26.0510 Anisotropy = 8.8902  
 XX= 28.3792 YX= -3.2317 ZX= 4.6542  
 XY= -3.3057 YY= 25.7295 ZY= 0.1838  
 XZ= 3.7487 YZ= 1.1462 ZZ= 24.0444  
 Eigenvalues: 20.4028 25.7726 31.9778  
 53 H Isotropic = 30.4612 Anisotropy = 5.9704  
 XX= 28.7590 YX= 0.3107 ZX= -2.6578  
 XY= 0.0104 YY= 32.4384 ZY= -2.5537  
 XZ= -2.0462 YZ= -2.4355 ZZ= 30.1862  
 Eigenvalues: 26.6435 30.2986 34.4415  
 54 H Isotropic = 29.4366 Anisotropy = 6.6558  
 XX= 31.9369 YX= -3.5647 ZX= 0.2802  
 XY= -3.5653 YY= 26.0163 ZY= 0.8501  
 XZ= -1.4340 YZ= 1.1906 ZZ= 30.3566  
 Eigenvalues: 24.2659 30.1700 33.8738  
 55 H Isotropic = 30.4634 Anisotropy = 8.0603  
 XX= 31.0539 YX= -0.1508 ZX= 1.0698  
 XY= 1.2331 YY= 26.8073 ZY= 4.1549  
 XZ= 2.8035 YZ= 2.8002 ZZ= 33.5290  
 Eigenvalues: 25.3195 30.2339 35.8370  
 56 H Isotropic = 28.9633 Anisotropy = 4.6145  
 XX= 30.1534 YX= -2.6535 ZX= -1.1976  
 XY= -2.4721 YY= 28.3285 ZY= 0.4301  
 XZ= 0.4970 YZ= 0.4255 ZZ= 28.4079  
 Eigenvalues: 26.5088 28.3414 32.0396  
 57 H Isotropic = 29.0736 Anisotropy = 5.1012  
 XX= 31.6927 YX= 0.1834 ZX= 0.2067  
 XY= 2.2520 YY= 30.3749 ZY= 1.7407  
 XZ= -0.7905 YZ= 1.5859 ZZ= 25.1531  
 Eigenvalues: 24.6123 30.1340 32.4744  
 58 H Isotropic = 27.3226 Anisotropy = 7.0079  
 XX= 27.5095 YX= -2.2352 ZX= -2.9248  
 XY= -2.1329 YY= 24.0814 ZY= 0.6884  
 XZ= -1.3732 YZ= 1.2324 ZZ= 30.3769  
 Eigenvalues: 23.0183 26.9550 31.9946  
 59 H Isotropic = 29.9742 Anisotropy = 6.1043  
 XX= 34.0348 YX= 0.4320 ZX= 0.1756  
 XY= 0.0380 YY= 27.7743 ZY= 1.7045  
 XZ= -0.3158 YZ= 0.8810 ZZ= 28.1134  
 Eigenvalues: 26.6334 29.2455 34.0437  
 60 H Isotropic = 29.6137 Anisotropy = 9.3462  
 XX= 26.8037 YX= 0.4007 ZX= -1.1519  
 XY= 0.9006 YY= 31.3148 ZY= -4.1660  
 XZ= -1.9129 YZ= -4.9508 ZZ= 30.7227  
 Eigenvalues: 25.8327 27.1640 35.8446  
 61 H Isotropic = 26.5947 Anisotropy = 3.3111  
 XX= 27.1223 YX= -1.4857 ZX= 1.8686  
 XY= -0.0948 YY= 28.4114 ZY= 1.4720  
 XZ= 2.7377 YZ= 0.3704 ZZ= 24.2503  
 Eigenvalues: 22.7232 28.2587 28.8021  
 62 H Isotropic = 30.6505 Anisotropy = 7.9222  
 XX= 34.6114 YX= 1.2530 ZX= 2.9938  
 XY= 0.1373 YY= 29.3466 ZY= -2.0649

XZ= 3.4706 YZ= -2.1610 ZZ= 27.9936  
 Eigenvalues: 25.4216 30.5980 35.9320  
 63 H Isotropic = 31.0979 Anisotropy = 7.7510  
 XX= 30.9978 YX= -0.8053 ZX= -0.7506  
 XY= -0.3861 YY= 32.7767 ZY= -4.9781  
 XZ= -0.8156 YZ= -4.7239 ZZ= 29.5191  
 Eigenvalues: 25.8430 31.1854 36.2652  
 64 H Isotropic = 30.1797 Anisotropy = 8.9310  
 XX= 28.4814 YX= -3.2533 ZX= -1.9934  
 XY= -3.6103 YY= 33.4749 ZY= 2.7792  
 XZ= -1.5034 YZ= 1.3122 ZZ= 28.5827  
 Eigenvalues: 26.4425 27.9628 36.1337  
 65 H Isotropic = 26.7637 Anisotropy = 2.9709  
 XX= 28.0002 YX= 0.8687 ZX= -0.5978  
 XY= 0.8259 YY= 27.5940 ZY= 0.9425  
 XZ= 0.1935 YZ= 1.2382 ZZ= 24.6968  
 Eigenvalues: 24.2731 27.2737 28.7443  
 66 H Isotropic = 30.3583 Anisotropy = 17.1304  
 XX= 39.6059 YX= 0.8127 ZX= 4.1583  
 XY= 1.7376 YY= 20.9649 ZY= 4.3851  
 XZ= 4.7180 YZ= 3.7198 ZZ= 30.5039  
 Eigenvalues: 19.4698 29.8265 41.7785  
 67 H Isotropic = 26.0727 Anisotropy = 9.8620  
 XX= 28.3307 YX= 5.3319 ZX= -0.1147  
 XY= 4.4251 YY= 26.9987 ZY= -0.2990  
 XZ= -0.9332 YZ= -0.8058 ZZ= 22.8887  
 Eigenvalues: 22.7013 22.8695 32.6474  
 68 H Isotropic = 29.5819 Anisotropy = 9.1609  
 XX= 35.3374 YX= 2.4818 ZX= 0.9277  
 XY= 0.0771 YY= 28.9801 ZY= -0.0746  
 XZ= 1.0723 YZ= 1.1188 ZZ= 24.4281  
 Eigenvalues: 24.3011 28.7553 35.6891  
 69 H Isotropic = 30.1650 Anisotropy = 7.1740  
 XX= 32.2057 YX= 0.7050 ZX= -1.9202  
 XY= 1.7506 YY= 33.6812 ZY= -1.0888  
 XZ= -1.9222 YZ= -2.2679 ZZ= 24.6080  
 Eigenvalues: 23.9573 31.5900 34.9476  
 70 H Isotropic = 30.1739 Anisotropy = 6.9316  
 XX= 30.1592 YX= 1.0035 ZX= -2.8106  
 XY= 1.4501 YY= 27.4510 ZY= 2.2191  
 XZ= -2.4934 YZ= 2.3919 ZZ= 32.9114  
 Eigenvalues: 25.5629 30.1638 34.7950  
 71 H Isotropic = 29.8417 Anisotropy = 7.2538  
 XX= 34.6034 YX= -0.0023 ZX= -0.1994  
 XY= 1.1737 YY= 30.0388 ZY= -2.4901  
 XZ= 0.8445 YZ= -3.2324 ZZ= 24.8829  
 Eigenvalues: 23.5837 31.2638 34.6775  
 72 H Isotropic = 29.4011 Anisotropy = 5.6430  
 XX= 31.9783 YX= 3.3416 ZX= -1.1384  
 XY= 2.5999 YY= 25.6947 ZY= 1.3984  
 XZ= -0.3346 YZ= 1.8792 ZZ= 30.5303  
 Eigenvalues: 24.0179 31.0224 33.1631  
 73 H Isotropic = 28.4868 Anisotropy = 4.2310  
 XX= 30.3788 YX= -0.9932 ZX= -0.5127  
 XY= -0.9129 YY= 29.4490 ZY= 0.9219

XZ= -1.1569 YZ= 1.5293 ZZ= 25.6326  
 Eigenvalues: 25.2147 28.9382 31.3075  
 74 H Isotropic = 30.3342 Anisotropy = 20.1966  
 XX= 39.1089 YX= 9.0262 ZX= 2.3315  
 XY= 9.7087 YY= 23.5050 ZY= 1.1520  
 XZ= 0.1816 YZ= 3.5972 ZZ= 28.3888  
 Eigenvalues: 18.8368 28.3673 43.7987  
 75 H Isotropic = 30.8812 Anisotropy = 7.6798  
 XX= 28.9894 YX= 1.5770 ZX= -1.5261  
 XY= 1.2057 YY= 28.1989 ZY= 2.3212  
 XZ= -1.5521 YZ= 0.7914 ZZ= 35.4553  
 Eigenvalues: 26.6139 30.0287 36.0011  
 76 H Isotropic = 30.0055 Anisotropy = 8.6837  
 XX= 31.4108 YX= 2.7925 ZX= 1.1072  
 XY= 3.0756 YY= 31.3727 ZY= 3.2643  
 XZ= 2.0584 YZ= 3.4807 ZZ= 27.2329  
 Eigenvalues: 25.3452 28.8766 35.7946  
 77 H Isotropic = 31.2613 Anisotropy = 8.1093  
 XX= 30.8244 YX= -2.4680 ZX= -0.3577  
 XY= -3.1751 YY= 35.0010 ZY= 0.9399  
 XZ= -0.5654 YZ= 1.8617 ZZ= 27.9584  
 Eigenvalues: 27.6871 29.4292 36.6675  
 78 H Isotropic = 30.0529 Anisotropy = 7.6191  
 XX= 27.2839 YX= 0.6684 ZX= -2.2790  
 XY= 0.8281 YY= 28.7155 ZY= 1.0755  
 XZ= -2.2508 YZ= 2.2036 ZZ= 34.1593  
 Eigenvalues: 26.0344 28.9920 35.1323  
 79 H Isotropic = 31.3446 Anisotropy = 8.8723  
 XX= 29.3941 YX= -1.5694 ZX= 0.6042  
 XY= -1.7119 YY= 33.4341 ZY= -4.3719  
 XZ= 0.8410 YZ= -4.4602 ZZ= 31.2056  
 Eigenvalues: 27.6317 29.1427 37.2595  
 80 H Isotropic = 30.5278 Anisotropy = 9.4470  
 XX= 34.0693 YX= 3.8775 ZX= -0.8814  
 XY= 3.7322 YY= 29.0610 ZY= -2.5976  
 XZ= -1.6197 YZ= -2.8075 ZZ= 28.4530  
 Eigenvalues: 25.6195 29.1381 36.8258  
 81 H Isotropic = 27.9986 Anisotropy = 5.6069  
 XX= 31.0129 YX= 1.6630 ZX= -1.1847  
 XY= 1.7614 YY= 25.6089 ZY= -2.1935  
 XZ= 0.2927 YZ= -1.5233 ZZ= 27.3740  
 Eigenvalues: 24.2066 28.0527 31.7366  
 82 H Isotropic = 32.0330 Anisotropy = 17.9562  
 XX= 38.3793 YX= -6.0153 ZX= 6.4594  
 XY= -4.8836 YY= 31.9119 ZY= -3.0907  
 XZ= 5.8733 YZ= -2.6128 ZZ= 25.8079  
 Eigenvalues: 23.2372 28.8581 44.0039  
 83 H Isotropic = 31.1303 Anisotropy = 9.7535  
 XX= 31.6944 YX= -4.2110 ZX= 1.9436  
 XY= -4.4872 YY= 34.0358 ZY= -1.1498  
 XZ= 0.9332 YZ= -0.7241 ZZ= 27.6608  
 Eigenvalues: 27.1376 28.6207 37.6327  
 84 H Isotropic = 30.4392 Anisotropy = 6.3721  
 XX= 29.5820 YX= -1.7925 ZX= -2.9303  
 XY= -2.4962 YY= 29.3958 ZY= 0.9458

XZ= -3.0285 YZ= -0.1790 ZZ= 32.3399  
Eigenvalues: 26.6402 29.9901 34.6873  
85 H Isotropic = 29.8258 Anisotropy = 7.4906  
XX= 33.7140 YX= 0.8437 ZX= 1.3703  
XY= 1.6238 YY= 31.5113 ZY= 1.8907  
XZ= 1.8763 YZ= 2.4376 ZZ= 24.2522  
Eigenvalues: 23.5014 31.1565 34.8196  
86 O Isotropic = -91.8301 Anisotropy = 613.7073  
XX= -175.2098 YX= -136.3230 ZX= -188.5731  
XY= -136.5793 YY= -257.6144 ZY= 156.8381  
XZ= -175.5071 YZ= 188.5481 ZZ= 157.3339  
Eigenvalues: -361.9318 -230.8666 317.3081

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