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$^1$H and $^{13}$C NMR of new compounds

(P,1S,2S)-1
(P,1S,2S)-3

R₂ = \text{phenyl acetate}
(P, 1S, 2S)-6

1H NMR (400 MHz, CDCl3)

13C NMR (100 MHz, CDCl3)
VT $^1$H-NMR of new compounds (P,1S,2S)-2-3 (500 MHz, CD$_2$Cl$_2$)

Compound (P,1S,2S)-2

Compound (P,1S,2S)-3
HPLC traces for compounds (P,1S,2S)-2-3

HPLC analysis were carried out on an Agilent 1260 series using the following conditions: CHIRALPAK® IC analytical column (4.6x250mm) packed with cellulose tris-(3,5-dichlorophenylcarbamate) immobilized on silica gel (5µm). The column temperature was set at 20 °C. The flow was constant during operation (1 mL/min) and 300 nm was selected as reference wavelength for the peak detection. The mobile phase gradient used is shown below:

| t (min) | Hexane | DCM |
|--------|--------|-----|
| 0      | 90     | 10  |
| 3      | 85     | 15  |
| 6      | 80     | 20  |
| 9      | 70     | 30  |
| 12     | 60     | 40  |
| 15     | 50     | 50  |
| 18     | 40     | 60  |
| 21     | 20     | 80  |
| 24     | 20     | 80  |
| 25     | 40     | 60  |
| 26     | 50     | 50  |
| 27     | 60     | 40  |
| 28     | 70     | 30  |
| 29     | 80     | 20  |

Figure S1. Chromatograms of (P,S,S)-2 (a) and (P,S,S)-3 (b).

a)
**ABSORPTION AND EXCITATION SPECTRA**

**Figure S2.** Excitation spectra of (P,S,S)-2 (A) and (P,S,S)-3 (B) at a concentration of 3.3 microM in different solvents. The emission wavelength was 475 nm.

**Figure S3.** Excitation spectra of (P,S,S)-2 (A) and (P,S,S)-3 (B) in CH₂Cl₂:Acetone (9:1), in the presence of increasing amounts of Ag(I). The emission wavelength was 475 nm.
**STEADY-STATE FLUORESCENCE SPECTRA**

**Figure S4.** Emission spectra of compounds (P,S,S)-2-3 in CH$_2$Cl$_2$ at $\lambda_{exc}$ = 300, 330, 340 and 350 nm.

![Emission spectra of compounds (P,S,S)-2-3 in CH$_2$Cl$_2$ at $\lambda_{exc}$ = 300, 330, 340 and 350 nm.](image)

**Figure S5.** Emission spectra of compound (P,S,S)-2 in different organic solvents at a) $\lambda_{exc}$ = 300 nm and (b) $\lambda_{exc}$ = 350 nm.

![Emission spectra of compound (P,S,S)-2 in different organic solvents at a) $\lambda_{exc}$ = 300 nm and (b) $\lambda_{exc}$ = 350 nm.](image)
Figure S6. Emission spectra of compound \((P,S,S)-3\) in different organic solvents at a) \(\lambda_{\text{exc}} = 300\) nm and (b) \(\lambda_{\text{exc}} = 350\) nm.
LIFETIMES, QUANTUM YIELDS AND TRES DECONVOLUTION OF COMPOUNDS (P,1S,2S)-2-3

Quantum yields were determined by measuring both absorbance and fluorescence of compounds (P,S,S)-2-3 and quinine in 0.1 M H₂SO₄ quinine sulphate as standard (Φᵣ = 0.54). For the relative determination of the fluorescence quantum yield Φ in a series of solvents, the following formula was used:

\[ \Phi_x = \Phi_r \frac{F_x}{F_r} \times \frac{1 - 10^{-A_x(\lambda_ex)}}{1 - 10^{-A_r(\lambda_ex)}} \times \frac{n^2_x}{n^2_r} \]

(eq. S1)

The subscripts \( x \) and \( r \) refer respectively to sample and reference (standard) fluorophore with known quantum yield \( \Phi_r \) in a specific solvent; \( F \) stands for the spectrally corrected, integrated fluorescence spectra; \( A(\lambda_ex) \) denotes the absorbance at the used excitation wavelength \( \lambda_ex \); and \( n \) represents the refractive index of the solvent (in principle at the average emission wavelength). To minimize inner filter effects, the absorbance at the excitation wavelength \( \lambda_ex \) was kept under 0.1. The measurements were performed using 10×10 mm cuvettes on non-degassed samples.

The fluorescence decay traces were fitted to a three/ four-exponential function, by using a Levenberg-Marquard algorithm-based nonlinear least-squares error minimization deconvolution method iterative deconvolution methods (FluoFit 4.4 package, Picoquant GmbH). For each sample, the decay traces were fitted globally with the decay times linked as shared parameters, whereas the pre-exponential factors were local adjustable parameters. The quality of fittings was assessed by the value of the reduced chi-squared, \( \chi^2 \), parameter and random distributions of the weighted residuals and the autocorrelation functions.

For the TRES (Time Resolved Emission Spectroscopy) analysis and the estimation of the species-associated emission spectra (SAEMS), the fitting procedure described above was performed, by fitting globally the 66 decay traces. The SAEMS of each species \( i \) at any given emission wavelength (SAEMS(\( \lambda_em \))) is given by the fluorescence intensity emitted by the species \( i \) (\( A_{i,\lambda_em} \times \tau_i \)), normalized by the total intensity and corrected for the different detection sensitivity using the total intensity of the steady-state spectrum (\( I_{ss,\lambda_em} \)):

\[ \text{SAEMS}(\lambda_{em}) = \frac{A_{i,\lambda_em} \times \tau_i}{\sum_i A_{i,\lambda_em} \times \tau_i} \cdot I_{ss,\lambda_em} \]

(eq. S2)
The approximate contribution of each species can be assessed as the area under the SAEMS. This estimation assumes equal excitation rate for all the species, as the initial amount of each form in the excited state (after the pulse excitation) is unknown. Figures 2b and 3b in main text show the SAEMS of compounds \((P,1S,2S)-2-3\) dissolved in dichloromethane.

**Table S1.** Quantum yields of compounds \((P,1S,2S)-2-3\) in different organic solvents.

| SOLVENT             | \((P,S,S)-2\)          | \((P,S,S)-3\)          |
|---------------------|------------------------|------------------------|
| Dichloromethane     | 0.55±0.09              | 0.44±0.03              |
| Acetonitrile        | 0.32±0.07              | 0.23±0.01              |
| Acetone             |                        | 0.27±0.01              |
| THF                 | 0.27±0.03              | 0.39±0.11              |
| Diethyl ether       | 0.37±0.03              | 0.40±0.04              |
| Ethyl acetate       | 0.27±0.05              | 0.34±0.02              |
| Methanol            | 0.30±0.06              | 0.18±0.02              |
| Hexane              | 0.14±0.04              | 0.42±0.03              |
| Toluene             | 0.29±0.06              | 0.47±0.02              |

**Table S2.** Lifetimes of compounds \((P,S,S)-2\) in different organic solvents determined at the maximum of emission of pyrene/helix (average of measurements at 398, 400 and 402 nm) and excimer-type (average of measurements at 536, 538 and 540 nm).

| SOLVENT       | \(\tau_1\) (ns) | \(\tau_2\) (ns) | \(\tau_3\) (ns) | \(\tau_4\) (ns) |
|---------------|----------------|----------------|----------------|----------------|
| Dichloromethane* | 23.49±0.27    | 7.705±0.032    | 2.007±0.047    | 0.454±0.039    |
| Acetonitrile     | 14.69±0.20    | 7.125±0.026    | 2.4727±0.056   | 0.909±0.075    |
| Acetone          | 15.33±0.37    | 7.638±0.027    | 2.376±0.051    | 1.0±0.2        |
| THF              | 20.11±0.31    | 7.837±0.036    | 2.37±0.047     | 1.00±0.12      |
| Diethyl ether    | 16.14±0.10    | 6.23±0.16      | 2.447±0.054    | 1.000±0.068    |
| Ethyl acetate    | 14.89±0.13    | 6.882±0.04     | 2.134±0.036    | 0.465±0.034    |
| Methanol         | 19.37±0.16    | 8.042±0.045    | 2.224±0.051    | 1.00±0.12      |
| Hexane           | 14.27±0.25    | 8.142±0.058    | 2.224±0.038    | 0.428±0.012    |
| Toluene          | 17.52±0.16    | 7.267±0.052    | 3.970±0.026    | 1.762±0.032    |
* As can be seen, lifetime of 21 ns (obtained in TRES deconvolution) is missing in this fitting. This can be justified considering the species that contributes to this time is neither present at 400 nor 540 nm, so it is not being observed when measuring at the maxima of emission.

**Table S3.** Lifetimes of compounds \((P,S,S)-3\) in different organic solvents determined at the maximum of emission of pyrene/helix (average of measurements at 398, 400 and 402 nm) and excimer-type (average of measurements at 536, 538 and 540 nm).

| SOLVENT         | \(\tau_1\) (ns) | \(\tau_2\) (ns) | \(\tau_3\) (ns) | \(\tau_4\) (ns) |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Dichloromethane | 35.43±0.16      | 7.11±0.11       | 4.56±0.080      | 0.515±0.019     |
| Acetonitrile    | 28.41±0.12      | 15.61±0.31      | 2.779±0.064     | 0.925±0.016     |
| Acetone         | 26.423±0.094    | 6.12±0.23       | 2.910±0.053     | 0.911±0.024     |
| THF             | 29.53±0.13      | 6.23±0.30       | 4.147±0.030     | 0.475±0.029     |
| Diethyl ether   | 42.87±0.22      | 6.89±0.23       | 4.535±0.034     | 0.421±0.041     |
| Ethyl acetate   | 28.07±0.13      | 7.13±0.46       | 4.006±0.028     | 0.403±0.027     |
| Methanol        | 26.056±0.096    | 10.34±0.49      | 1.704±0.040     | 0.696±0.013     |
| Hexane          | 33.85±0.17      | 7.31±0.50       | 4.306±0.029     | 0.606±0.06      |
| Toluene         | 28.447±0.092    | 9.92±0.92       | 3.750±0.028     | 0.442±0.021     |
**Figure S7.** Normalized emission spectra of (P,1S,2S)-2 at different times after a δ-pulse excitation.

**Figure S8.** Normalized emission spectra of (P,1S,2S)-3 at different times after a δ-pulse excitation.
**CD TITRATION OF COMPOUNDS (P,1S,2S)-2-3 WITH AgBF₄**

**General procedure for the CD-titration of compounds (P,1S,2S)-2-3**

**Figure S9.** CD titration of compound (P,1S,2S)-2 with AgBF₄ in CH₂Cl₂ as solvent.

The fitting was carried out with DynaFit program (v. 4.06019), which has been previously used to study guest-host complexation equilibria. ECD spectra showed in Figures S6 and S8 are an average spectra calculated after 30 scans (each one).

**Figure S10.** Dynafit analysis of CD titration of compound (P,1S,2S)-2.
Figure S11. CD titration of compound (P,1S,2S)-3 with AgBF₄ in CH₂Cl₂ as solvent.

Figure S12. Linear fitting of the ratio between absolute value of $\Delta \varepsilon$ intensity at 345 nm and 387 nm versus Ag(I) concentration for compound (P,1S,2S)-3 with AgBF₄.
Figure S13. Dynafit analysis of CD titration of compound (P,1S,2S)-3.

![Graph showing the Dynafit analysis of CD titration of compound (P,1S,2S)-3.]

### Parameters

#### Marquardt Algorithm

#### Optimized Parameters

| No | Par#Set | Initial | Final | Std. Error | CV (%) | Low(95) | High(95) | Note |
|----|---------|---------|-------|------------|--------|---------|----------|------|
| #1 | K       | 6360.95 | 6360  | 330        | 5.2    | 5710    | 7080     |      |
| #2 | r(L)    | 3.16244e+006 | 3.162e+006 | 14000   | 0.5    | 3.134e+006 | 3.192e+006 |      |
| #3 | r(LAg)  | 1.28413e+006 | 1.285e+006 | 26000   | 2.0    | 1.23e+006  | 1.336e+006 |      |

(95) Confidence intervals at 95% probability level.
**CPL MEASUREMENTS**

Experimental

CPL spectra in Figure S11 were collected by accumulating 150 scans and with 0.5 s of integration time. Some of the measurements were also carried out in a home-made apparatus,\(^5\) with the excitation radiation brought to the sample from a Jasco FP8200 fluorimeter through an optical fiber.

**Figure S14.** \(g_{\text{lum}}\) values obtained for compounds \((P,1S,2S)-2\) and \((P,1S,2S)-3\) in CH\(_2\)Cl\(_2\) as solvent in the absence and presence of Ag(I).

**Figure S15.** \(g_{\text{lum}}\) values obtained for compounds \((M,1R,2R)-2-3\) and \((P,1S,2S)-2-3\) in CH\(_2\)Cl\(_2\) as solvent.
THEORETICAL CALCULATIONS

Molecular mechanics (MM) conformational search have been performed for compounds \((P,S,S)\)-2-3 starting from both \(M\) and \(P\) structures. Conformers within 5 kcal/mol were all optimized at B3LYP/6-31g* level.

Populated conformers have been optimized also within the framework of polarizable continuum model approximation (PCM) CAM-B3LYP/6-31g*, checking that all structures correspond to minima and evaluating the Gibbs free energy.

From all structures thus obtained, a new optimization has been performed in presence of Ag (I).

The time-dependent DFT (TD-DFT) method has been used to calculate Absorption and CD spectra at the same level of approximation, namely iefpcm CAM-B3LYP/6-31G*.

All calculations have been performed with Gaussian09 package.\(^6\)
Table S4. Principal conformers of compound \((P,S,S)-2\) in absence and presence of Ag (OPE moiety conformation is 77\% P). Some dihedral angles are reported following the atom numbering of the figure below.

| Ag  | Keal | pop  | 55.56, 56.55, 56.59, 55.88, 61.60, 91.89, 43.35, 33.55, 35.50, 49.55, 36.49, 33.36, 32.33, 36.49 |
|-----|------|------|----------------------------------------------------------|
| a   | P    | sym  | -120, -118, -69, -88, -61, -61, -156, 67, 57, -176, 57, 67, -156 |
| b   | M    | 1.09 | -143, -144, -175, 177, -174, -67, -10, -166, 82, -50, 82, -167, -10 |
| c   | P    | 1.15 | -119, -116, -68, -68, -61, 123, -157, 63, 57, -176, 58, 66, -155 |
| d   | P    | 1.35 | -119, -141, -68, 174, -61, 68, -158, 67, 58, -176, 57, 67, 26 |
| e   | M    | 1.73 | -153, -147, -177, -176, 63, -70, -10, -167, 84, -51, 83, -167, -10 |
| f   | P    | 1.81 | -141, -147, -177, 75, -179, 64, -158, 68, 57, -173, 59, 67, -157 |
| g   | M    | 2.31 | -102, -152, -174, 177, -65, 69, -9, -167, 81, -51, 84, -166, -10 |

The figure below shows the atom numbering used to report the dihedral angles.
**Figure S16.** Four principal conformers of *P* type and three of *M* type of compound \((P,S,S)\)-2 (first row left: *P* conformers without Ag(I), right: conformers in presence of Ag(I); second row left: *M* conformers without Ag(I), right conformers in presence of Ag(I)).

**Figure S17.** First two conformations of compound \((P,S,S)\)-2 in absence (light blue) and presence (blue) of Ag(I).
**Figure S18.** Rotational strengths for the most populated conformers. Rotational strengths for some transitions are maintained also upon Ag(I) complexation (green circles), while other are switched off in the presence of Ag(I) (black circles). No wavelength shift has been applied.
Figure S19. Orbitals involved in the first principal transitions are reported for conformer a of compound \((P,S,S)-2\) in absence of Ag(I). In the table on the right the assignment of the lower energy transitions: orbitals localized on the pyrene rings are evidenced in green; among the others some are localized on the OPE backbone, but some are delocalized on the whole molecule. Differently from the case of the diester \((P,S,S)-3\), there is not a clear separation between the two moieties.
| state | mm      | C     | R     | Cl coeff |
|-------|---------|-------|-------|----------|
| 1     | 317     | 6.10E+05 | 1078     | 250 → 254 | -0.48 |
|       |         |       |       | 251 → 253 | 0.48  |
| 2     | 315     | 2.61E+05 | 1415     | 250 → 253 | -0.47 |
|       |         |       |       | 251 → 254 | 0.48  |
| 3     | 307     | 1.04E+03 | 3       | 246 → 254 | -0.28 |
|       |         |       |       | 247 → 253 | -0.25 |
|       |         |       |       | 248 → 253 | 0.22  |
|       |         |       |       | 249 → 254 | 0.19  |
|       |         |       |       | 250 → 260 | 0.33  |
|       |         |       |       | 251 → 261 | 0.36  |
| 4     | 307     | 1.18E+03 | 7       | 246 → 253 | 0.28  |
|       |         |       |       | 247 → 254 | 0.25  |
|       |         |       |       | 248 → 254 | -0.23 |
|       |         |       |       | 249 → 253 | -0.19 |
|       |         |       |       | 250 → 261 | 0.35  |
|       |         |       |       | 251 → 260 | 0.34  |
| 5     | 303     | 3.23E+05 | 76      | 245 → 252 | 0.46  |
|       |         |       |       | 247 → 252 | 0.34  |
|       |         |       |       | 248 → 252 | 0.34  |
| 6     | 204     | 2.02E+05 | -115    | 233 → 252 | 0.16  |
|       |         |       |       | 246 → 252 | 0.32  |
|       |         |       |       | 249 → 252 | 0.51  |
| 7     | 274     | 2.73E+04 | 271     | 245 → 252 | 0.33  |
|       |         |       |       | 246 → 256 | 0.17  |
|       |         |       |       | 247 → 255 | -0.25 |
|       |         |       |       | 249 → 252 | -0.19 |
|       |         |       |       | 248 → 255 | -0.30 |
|       |         |       |       | 249 → 256 | 0.26  |
| 8     | 263     | 2.07E+05 | -91     | 246 → 255 | 0.30  |
|       |         |       |       | 248 → 257 | 0.15  |
|       |         |       |       | 249 → 255 | 0.47  |
Figure S20. As an example the calculated ECD spectrum for the first conformer (a) of (P,S,S)-2 is reported below, with the principal orbitals involved in the transitions assigned to bands conserved upon Ag complexation (green arrows) and to the bands switched off upon Ag complexation (black arrows), complete CI results have been reported in the above table.
Table S5. Principal conformers of compound \((P,S,S)-3\) in absence and presence of \(\text{Ag}\) (\(\text{OPE}\) moiety conformation is 77% P). Some dihedral angles are reported following the atom numbering of the figure below. Upon \(\text{Ag(I)}\) addition, conformers \(b\) and \(d\) gave equivalent structures.

|        | \(\text{Kcal/mole}\) | \(\text{pop}\) | 92.90 | 90.88 | 88.87 | 87.55 | 56.59 | 55.56 | 56.59 | 59.85 | 62.60 | 85.60 | 85.59 | 34.33 | 33.36 | 36.43 | 49.55 | 56.50 | 55.56 | 56.50 | 35.3 | 3.4 |
|--------|------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| \(a\)  | 0.00                   | 33.5\%        | -9     | 177    | -152   | -51    | -152   | 177    | -9     | -167   | 69     | 58     | -170   | 58     | 69     | -167   |
| \(b\)  | 0.63                   | 23.0\%        | -13    | 174    | -150   | 57     | -107   | 180    | 12     | 177    | 80     | 66     | -68    | -55    | 160    | -164   |
| \(c\)  | 0.73                   | 19.5\%        | -152   | 177    | -154   | -51    | -153   | -177   | 23     | -167   | 69     | 58     | -169   | 58     | 69     | -166   |
| \(d\)  | 0.75                   | 18.9\%        | -9     | 177    | -104   | 57     | -150   | 176    | -11    | 15     | 160    | -55    | -68    | 66     | 80     | 177    |
| \(e\)  | 1.52                   | 5.1\%         | -12    | 176    | -150   | 59     | -109   | 179    | -163   | 177    | 80     | 66     | -66    | -57    | 159    | -164   |

| \(\text{Ag}\) | \(\text{Kcal/mole}\) | \(\text{pop}\) | 92.90 | 90.88 | 88.87 | 87.55 | 56.59 | 55.56 | 56.59 | 59.85 | 62.60 | 85.60 | 85.59 | 34.33 | 33.36 | 36.43 | 49.55 | 56.50 | 55.56 | 56.50 | 35.3 | 3.4 |
|--------------|------------------------|----------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| \(a\)  | 0.00                   | 64.4\%        | -6     | 177    | -151   | -60    | -151   | 177    | -6     | -173   | 72     | 53     | -179   | 53     | 72     | -173   |
| \(c\)  | 1.18                   | 17.8\%        | -155   | 178    | -154   | -58    | -151   | -177   | 23     | -174   | 72     | 54     | -177   | 53     | 72     | -174   |
| \(b,d\)| 1.24                   | 15.8\%        | 10     | 179    | -101   | 48     | -150   | 174    | -5     | 13     | 156    | -58    | -77    | 64     | 84     | 174    |
| \(e\)  | 2.39                   | 2.3\%         | -9     | 176    | -151   | 54     | -106   | 179    | -167   | 173    | 84     | 64     | -72    | -59    | 159    | -170   |
**Figure S21.** Main conformers of compound (P,S,S)-3 (left, without Ag(I), right, in the presence of Ag(I)).

**Figure S22.** First two conformations of compound (P,S,S)-3 in absence (light blue) and presence (blue) of Ag(I).
Figure S23. Rotational strengths for the most populated conformers. Rotational strengths for some transitions are maintained also upon Ag(I) complexation (green circles), while other are switched off in the presence of Ag(I) (black circles). No wavelength shift has been applied.
Figure S24. Orbitals involved in the first principal transitions are reported for conformer \textit{a} of compound $p$-($P,S,S$)-3 in absence of Ag(I). In the table, on the right the assignment of the lower energy transitions: orbitals localized on the pyrene rings are evidenced in green; among the others, some are localized on the OPE backbone, but some are delocalized on the whole molecule.
| state | n,m | D     | R   | Ci coeff. |
|-------|-----|-------|-----|-----------|
| 1     | 344 | 9.28E+05 | 166 | 256 -> 259 | 0.48 |
|       |     |        |     | 257 -> 260 | -0.48|
| 2     | 340 | 1.93E+05 | -283| 256 -> 260 | -0.48|
|       |     |        |     | 257 -> 259 | 0.48 |
| 3     | 314 | 3.88E+04 | -35 | 252 -> 259 | 0.40 |
|       |     |        |     | 253 -> 260 | -0.40|
|       |     |        |     | 256 -> 265 | 0.17 |
|       |     |        |     | 257 -> 266 | 0.17 |
| 4     | 314 | 5.66E+04 | 74  | 252 -> 260 | -0.39|
|       |     |        |     | 253 -> 259 | 0.39 |
|       |     |        |     | 256 -> 266 | 0.28 |
|       |     |        |     | 257 -> 265 | 0.27 |
| 5     | 306 | 2.63E+05 | 194 | 251 -> 258 | 0.35 |
|       |     |        |     | 255 -> 258 | 0.55 |
|       |     |        |     | 242 -> 258 | -0.17|
| 6     | 286 | 3.97E+05 | -211| 254 -> 258 | 0.61 |
|       |     |        |     | 255 -> 262 | -0.14|
| 7     | 274 | 1.01E+05 | 370 | 251 -> 258 | 0.44 |
|       |     |        |     | 254 -> 262 | 0.30 |
|       |     |        |     | 255 -> 258 | -0.18|
|       |     |        |     | 255 -> 261 | 0.33 |
| 8     | 286 | 2.11E+05 | -75 | 254 -> 261 | 0.36 |
|       |     |        |     | 255 -> 263 | 0.19 |
Figure S25. As an example, the calculated ECD spectrum for the first conformer (a) of (P,S,S)-3 is reported below, with the principal orbitals involved in the transitions assigned to bands conserved upon Ag complexation (green arrows) and to the bands switched off upon Ag complexation (black arrows), complete CI results have been reported in the above table.
Cartesian coordinates, computed total energies and lowest frequency values for the optimized structures discussed in text
Principal conformers of compound \(p-(P,S,S)-2\) in absence and presence of Ag.

\(p-(P,S,S)-2\): conformer \(a\)

### Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 6             | 0           | 2.385192 0.494100 -0.976149 |
| 2             | 6             | 0           | 2.470459 1.825256 -0.596083 |
| 3             | 6             | 0           | 1.277180 0.053307 -1.700197 |
| 4             | 6             | 0           | 0.281689 0.962118 -2.065871 |
| 5             | 6             | 0           | 0.371752 2.288012 -1.682403 |
| 6             | 6             | 0           | 1.464036 2.739559 -0.926928 |
| 7             | 1             | 0           | 3.175497 -0.187540 -0.688224 |
| 8             | 1             | 0           | 3.325590 2.158713 -0.017724 |
| 9             | 1             | 0           | -0.570069 0.602019 -2.632703 |
| 10            | 1             | 0           | -0.419396 2.982442 -1.943480 |
| 11            | 6             | 0           | 1.544219 4.089143 -0.466570 |
| 12            | 6             | 0           | 1.633269 5.217261 -0.039025 |
| 13            | 6             | 0           | 1.827558 6.533970 0.475889 |
| 14            | 6             | 0           | 3.105225 6.915637 0.907061 |
| 15            | 6             | 0           | 0.769064 7.465253 0.562044 |
| 16            | 6             | 0           | 3.339336 8.186345 1.408025 |
| 17            | 6             | 0           | 2.297312 9.106564 1.486731 |
| 18            | 6             | 0           | 1.026508 8.746838 1.066789 |
| 19            | 6             | 0           | -0.559689 7.143485 0.147508 |
| 20            | 6             | 0           | -1.710913 6.959630 -0.174010 |
| 21            | 6             | 0           | -3.074078 6.847467 -0.586345 |
| 22            | 6             | 0           | -3.719352 7.979579 -1.101463 |
| 23            | 6             | 0           | -5.040153 7.920804 -1.517235 |
| 24            | 6             | 0           | -5.743909 6.722468 -1.423824 |
| 25            | 6             | 0           | -5.123416 5.593427 -0.912963 |
| 26            | 6             | 0           | -3.789261 5.633592 -0.485955 |
| 27            | 6             | 0           | -3.192430 4.448692 0.039777 |
| 28            | 6             | 0           | -2.754602 3.409422 0.477372 |
| 29            | 6             | 0           | -2.255046 2.158139 0.950852 |
| 30            | 6             | 0           | -1.082108 2.081382 1.716611 |
| 31            | 6             | 0           | -2.917805 0.969995 0.623488 |
| 32            | 6             | 0           | -0.580815 0.855156 2.114064 |
| 33            | 6             | 0           | -1.234688 -0.324706 1.751661 |
| 34            | 6             | 0           | -2.419176 -0.262891 1.017181 |
| 35            | 8             | 0           | 1.087591 -1.239118 -2.098737 |
| 36            | 8             | 0           | -0.648073 -1.487050 2.163136 |
| 37            | 1             | 0           | 3.913611 6.195833 0.839119 |
| 38            | 1             | 0           | 4.337380 8.460370 1.735681 |
| 39            | 1             | 0           | 2.474661 10.103483 1.876377 |
| 40            | 1             | 0           | 0.208296 9.456155 1.127176 |
| 41            | 1             | 0           | -3.163329 8.908018 -1.172794 |
| 42            | 1             | 0           | -5.520563 8.808692 -1.914720 |
| 43            | 1             | 0           | -6.778068 6.668787 -1.747764 |
| 44            | 1             | 0           | -5.666955 4.658287 -0.833688 |
| 45            | 1             | 0           | -0.552668 2.992323 1.973914 |
| 46 | 1 | 0 | -3.829251 | 1.011235 | 0.036624 |
|---|---|---|-----------|---------|---------|
| 47 | 1 | 0 | 0.336439  | 0.786623 | 2.688966 |
| 48 | 1 | 0 | -2.950788 | -1.161822| 0.731433 |
| 49 | 6 | 0 | -0.926351 | -2.689184| 1.447953 |
| 50 | 6 | 0 | 1.726760  | -2.85427 | -1.369498|
| 51 | 1 | 0 | -1.998505 | -2.899455| 1.414651 |
| 52 | 1 | 0 | -0.443663 | -3.484490| 2.017238 |
| 53 | 1 | 0 | 1.519182  | -3.198305| -1.929189|
| 54 | 1 | 0 | 2.810807  | -2.148932| -1.336001|
| 55 | 6 | 0 | -0.348466 | -2.650181| 0.033951 |
| 56 | 6 | 0 | -0.443663 | -3.484490| 2.017238 |
| 57 | 1 | 0 | -0.809953 | -1.827348| 0.044785 |
| 58 | 1 | 0 | 1.345320  | -1.480551| 0.590020 |
| 59 | 8 | 0 | 1.820402  | -3.492082| 0.686471 |
| 60 | 6 | 0 | 3.818113  | -2.323804| 1.547052 |
| 61 | 6 | 0 | 4.857169  | -2.827917| 0.738692 |
| 62 | 6 | 0 | 3.945464  | -1.055956| 2.108464 |
| 63 | 6 | 0 | 5.071370  | -0.272228| 1.893355 |
| 64 | 6 | 0 | 6.118320  | -0.740956| 1.099733 |
| 65 | 6 | 0 | 6.014281  | -2.033187| 0.516512 |
| 66 | 6 | 0 | 4.797467  | -4.131630| 0.126557 |
| 67 | 6 | 0 | 7.084014  | -2.529876| -0.290030|
| 68 | 6 | 0 | 6.996173  | -3.820381| -0.872383|
| 69 | 6 | 0 | 5.813863  | -4.600445| -0.633703|
| 70 | 6 | 0 | 7.301567  | 0.041937 | 0.856847 |
| 71 | 6 | 0 | 8.310031  | -0.430220| 0.912283 |
| 72 | 6 | 0 | 8.240546  | -1.735604| -0.511007|
| 73 | 6 | 0 | 9.274311  | -2.242205| -1.302233|
| 74 | 6 | 0 | 9.180119  | -3.507638| -1.869340|
| 75 | 6 | 0 | 8.053476  | -4.290428| -1.657784|
| 76 | 1 | 0 | 3.142732  | -0.673949| 2.733295 |
| 77 | 1 | 0 | 5.143731  | -0.712537| 2.345603 |
| 78 | 1 | 0 | 3.906057  | -4.730680| 0.265811 |
| 79 | 1 | 0 | 5.748901  | -5.585962| -1.085948|
| 80 | 1 | 0 | 7.364780  | 1.027779 | 1.308211|
| 81 | 1 | 0 | 9.198208  | 0.169920 | -0.083856|
| 82 | 1 | 0 | 10.158167 | -1.633712| -1.470522|
| 83 | 1 | 0 | 9.992881  | -3.885786| -2.481267|
| 84 | 1 | 0 | 7.983382  | -5.278731| -2.102801|
| 85 | 6 | 0 | 2.580766  | -3.140628| 1.840260 |
| 86 | 1 | 0 | 1.947836  | -2.595371| 2.550525 |
| 87 | 1 | 0 | 2.847948  | -4.097072| 2.298506 |
| 88 | 8 | 0 | -0.645750 | -3.889472| -0.589602|
| 89 | 6 | 0 | -2.860092 | -3.396000| -1.535799|
| 90 | 6 | 0 | -3.308179 | -2.178552| -2.160119|
| 91 | 6 | 0 | -3.747392 | -4.070480| -0.719916|
| 92 | 6 | 0 | -5.081318 | -3.608379| -0.554189|
| 93 | 6 | 0 | -5.512877 | -2.418759| -1.207151|
| 94 | 6 | 0 | -4.608871 | -1.719443| -2.001376|
| 95 | 6 | 0 | -3.356756 | -5.282832| -0.044994|
| 96 | 6 | 0 | -4.230154 | -5.974616| 0.722840 |
| 97 | 6 | 0 | -5.584420 | -5.532064| 0.906486 |
| 98 | 6 | 0 | -5.999926 | -4.339858| 0.259894 |
| 99 | 6 | 0 | -6.869481 | -1.974732| -1.015758|
|100 | 6 | 0 | -7.734614 | -2.667828| -0.242959|
101  6  0  -7.333136  -3.878308  0.424164
102  6  0  -8.213827  -4.609934  1.224433
103  6  0  -7.798339  -5.776634  1.855216
104  6  0  -6.497372  -6.234913  1.699092
105  6  0  -1.440044  -3.801371  -1.770435
106  1  0  -4.930518  -0.811037  -2.502236
107  1  0  -2.334070  -5.625366  -0.143601
108  1  0  -3.915430  -6.886167  1.222846
109  1  0  -7.183124  -1.063202  -1.516126
110  1  0  -8.756020  -2.322893  -0.111028
111  1  0  -9.233033  -4.255945  1.349531
112  1  0  -8.495854  -6.332719  2.473494
113  1  0  -6.176347  -7.147141  2.193566
114  1  0  -1.425341  -4.811354  -2.189790
115  1  0  -0.959270  -3.131944  -2.493667
116  1  0  -2.620372  -1.621364  -2.790171

SCF Done:  E(RCAM-B3LYP) =  -2916.94878205
Full mass-weighted force constant matrix:
Low frequencies ---  -0.0017  -0.0009  0.0007  0.2645  1.6788
4.3025
Low frequencies ---  5.8831  6.9871  8.6807
### Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -3.362030  | -0.574343  | -1.498619   |
| 2             | 6             | 0           | -4.673291  | -0.997543  | -1.413799   |
| 3             | 6             | 0           | -2.382605  | -1.151125  | -0.685080   |
| 4             | 6             | 0           | -2.717331  | -2.202461  | 0.166615    |
| 5             | 6             | 0           | -4.038042  | -2.626102  | 0.242482    |
| 6             | 6             | 0           | -5.037924  | -2.020415  | -0.523850   |
| 7             | 1             | 0           | -3.077189  | 0.232503   | -2.164457   |
| 8             | 1             | 0           | -5.435191  | -0.523460  | -2.022882   |
| 9             | 1             | 0           | -1.967947  | -2.686417  | 0.780361    |
| 10            | 1             | 0           | -4.301517  | -3.41093   | 0.920320    |
| 11            | 6             | 0           | -6.400023  | -2.425653  | -0.374331   |
| 12            | 6             | 0           | -7.544724  | -2.775104  | -0.199814   |
| 13            | 6             | 0           | -8.851369  | -3.307912  | 0.020343    |
| 14            | 6             | 0           | -8.986025  | -4.684982  | 0.245523    |
| 15            | 6             | 0           | -10.007944 | -2.498197  | 0.023101    |
| 16            | 6             | 0           | -10.228935 | -5.257472  | 0.463472    |
| 17            | 6             | 0           | -11.370654 | -4.459806  | 0.459143    |
| 18            | 6             | 0           | -11.257549 | -3.096384  | 0.240799    |
| 19            | 6             | 0           | -9.969694  | -1.085019  | -0.188573   |
| 20            | 6             | 0           | -10.084873 | 0.108727   | -0.349350   |
| 21            | 6             | 0           | -10.387104 | 1.486062   | -0.583961   |
| 22            | 6             | 0           | -11.694203 | 1.815871   | -0.970499   |
| 23            | 6             | 0           | -12.056959 | 3.129176   | -1.221641   |
| 24            | 6             | 0           | -11.113904 | 4.145530   | -1.089446   |
| 25            | 6             | 0           | -9.818687  | 3.839520   | -0.703610   |
| 26            | 6             | 0           | -9.433078  | 2.517258   | -0.443003   |
| 27            | 6             | 0           | -8.084427  | 2.262044   | -0.048822   |
| 28            | 6             | 0           | -6.924685  | 2.149310   | 0.275501    |
| 29            | 6             | 0           | -5.539256  | 2.024569   | 0.602189    |
| 30            | 6             | 0           | -4.592168  | 2.829234   | -0.037635   |
| 31            | 6             | 0           | -5.092694  | 1.081934   | 1.542060    |
| 32            | 6             | 0           | -3.233806  | 2.676437   | 0.209252    |
| 33            | 6             | 0           | -2.805748  | 1.700570   | 1.107776    |
| 34            | 6             | 0           | -3.744792  | 0.927901   | 1.797031    |
| 35            | 8             | 0           | -1.136921  | -0.616051  | -0.783989   |
| 36            | 8             | 0           | -1.501005  | 1.422685   | 1.367920    |
| 37            | 1             | 0           | -8.092915  | -5.300200  | 0.243276    |
| 38            | 1             | 0           | -10.307739 | -6.326034  | 0.634557    |
| 39            | 1             | 0           | -12.347988 | -4.900036  | 0.627070    |
| 40            | 1             | 0           | -12.141082 | -2.467427  | 0.238888    |
| 41            | 1             | 0           | -12.421405 | 1.017979   | -1.074241   |
| 42            | 1             | 0           | -13.073815 | 3.360023   | -1.521485   |
| 43            | 1             | 0           | -11.388738 | 5.176808   | -1.285053   |
| 44            | 1             | 0           | -9.079881  | 4.625924   | -0.594630   |
| 45            | 1             | 0           | -4.923508  | 3.575069   | -0.752369   |
| 46            | 1             | 0           | -5.815178  | 0.456065   | 2.054391    |
| 47            | 1             | 0           | -2.524693  | 3.307740   | -0.311442   |
| 48            | 1             | 0           | -3.390725  | 0.184032   | 2.501831    |
| 49            | 6             | 0           | -0.503565  | 2.013685   | 0.547074    |
|    | 6  | 0  | -0.156091 | -0.997128 | 0.169692 |
|----|----|----|-----------|-----------|----------|
| 50 |    |    |           |           |          |
| 51 |    |    | -0.392573 | 3.075609  | 0.794562 |
| 52 |    |    | -0.776639 | 1.929134  | -0.508757|
| 53 |    |    | -0.577791 | -0.987733 | 1.178905 |
| 54 |    |    | 0.207618  | -2.008258 | -0.046719|
| 55 |    |    | 1.011325  | -0.016723 | 0.069077 |
| 56 |    |    | 0.890908  | 1.092381  | 1.894945 |
| 57 |    |    |           |           |          |
| 58 |    |    | 1.184557  | 0.219497  | -0.988909|
| 59 | 8  | 0  | 2.158905  | -0.630295 | 0.633634 |
| 60 |    |    | 4.091285  | -2.027559 | 0.409773 |
| 61 |    |    | 5.100800  | -2.668204 | -0.334526|
| 62 |    |    | 4.135712  | -2.063731 | 1.799350 |
| 63 |    |    | 5.163089  | -2.713318 | 2.470646 |
| 64 |    |    | 5.184391  | -3.352452 | 1.769149 |
| 65 |    |    | 6.154718  | -3.323240 | 0.348939 |
| 66 |    |    | 5.112438  | -2.679933 | -1.775608|
| 67 |    |    | 7.192108  | -3.983451 | -0.386960|
| 68 |    |    | 7.173933  | -3.973194 | -1.805663|
| 69 |    |    | 6.094546  | -3.298387 | -2.471083|
| 70 |    |    | 7.264872  | -4.030616 | 2.435754 |
| 71 |    |    | 8.245767  | -4.644364 | 1.737578 |
| 72 |    |    | 8.246854  | -4.644320 | 0.298111 |
| 73 |    |    | 9.251069  | -5.272784 | -0.442319|
| 74 |    |    | 9.225801  | -5.257114 | -1.831897|
| 75 |    |    | 8.198326  | -4.614737 | -2.509010|
| 76 | 1  | 0  | 3.350583  | -1.569509 | 2.351724 |
| 77 | 1  | 0  | 5.176089  | -2.724953 | 3.556711 |
| 78 | 1  | 0  | 4.315002  | -2.182722 | -2.316554|
| 79 | 1  | 0  | 6.082158  | -3.293685 | -3.557175|
| 80 | 1  | 0  | 7.273008  | -4.036391 | 3.521921 |
| 81 | 1  | 0  | 9.056252  | -5.152294 | 2.252221 |
| 82 | 1  | 0  | 10.057269 | -5.777337 | 0.082366 |
| 83 | 1  | 0  | 10.014543 | -5.750708 | -2.390810|
| 84 | 1  | 0  | 8.181524  | -4.604864 | -3.594976|
| 85 | 6  | 0  | 2.971034  | -1.309299 | -0.302590|
| 86 | 1  | 0  | 2.370835  | -2.029668 | -0.878866|
| 87 | 1  | 0  | 3.378845  | -0.582827 | -1.019356|
| 88 | 8  | 0  | 1.881648  | 2.142690  | 0.404366 |
| 89 | 6  | 0  | 3.557633  | 3.774652  | 0.894002 |
| 90 | 6  | 0  | 3.449339  | 5.155899  | 0.765724 |
| 91 | 6  | 0  | 4.762110  | 3.137952  | 0.538106 |
| 92 | 6  | 0  | 5.849142  | 3.922575  | 0.067204 |
| 93 | 6  | 0  | 5.715366  | 5.332132  | -0.052576|
| 94 | 6  | 0  | 4.504806  | 5.928013  | 0.301227 |
| 95 | 6  | 0  | 4.942119  | 1.711710  | 0.640326 |
| 96 | 6  | 0  | 6.116266  | 1.125325  | 0.310254 |
| 97 | 6  | 0  | 7.233227  | 1.893785  | -0.165259|
| 98 | 6  | 0  | 7.085726  | 3.299597  | -0.285250|
| 99 | 6  | 0  | 8.633204  | 6.101041  | -0.533367|
| 100| 6  | 0  | 8.000923  | 5.508364  | -0.867769|
| 101| 6  | 0  | 8.172621  | 4.083788  | -0.755337|
| 102| 6  | 0  | 9.372481  | 3.452658  | -1.093016|
| 103| 6  | 0  | 9.508352  | 2.074671  | -0.973324|
| 104| 6  | 0  | 8.450679  | 1.301099  | -0.514486|
|   |   |   |   |   |
|---|---|---|---|---|
|105| 6 | 0 | 2.393300| 2.986430| 1.429413|
|106| 1 | 0 | 4.393824| 7.004641| 0.211711|
|107| 1 | 0 | 4.106991| 1.101401| 0.963559|
|108| 1 | 0 | 6.230439| 0.048444| 0.394942|
|109| 1 | 0 | 6.714628| 7.177158| -0.621021|
|110| 1 | 0 | 8.837168| 6.099987| -1.229052|
|111| 1 | 0 | 10.203205| 4.053354| -1.452147|
|112| 1 | 0 | 10.447459| 1.600480| -1.240550|
|113| 1 | 0 | 8.559674| 0.224204| -0.423530|
|114| 1 | 0 | 1.616892| 3.675571| 1.786086|
|115| 1 | 0 | 2.700127| 2.367823| 2.284499|
|116| 1 | 0 | 2.515932| 5.639071| 1.040098|

SCF Done:  E(RCAM-B3LYP) = -2916.94704596
Full mass-weighted force constant matrix:
Low frequencies ---  -1.9049  -1.6315  -0.0025  -0.0010  -0.0006
2.3833
Low frequencies ---  6.6331  7.6971  9.0762
**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 2.016675    | 0.838220    | -0.852453   |
| 2             | 6             | 0           | 1.523122    | 2.108808    | -0.592917   |
| 3             | 6             | 0           | 1.161501    | -0.145112   | -1.350737   |
| 4             | 6             | 0           | -0.173229   | 0.166976    | -1.618229   |
| 5             | 6             | 0           | -0.658514   | 1.434836    | -1.356782   |
| 6             | 6             | 0           | 0.180067    | 2.425404    | -0.824415   |
| 7             | 1             | 0           | 3.058061    | 0.626486    | -0.644855   |
| 8             | 1             | 0           | 2.180017    | 2.863364    | -0.186084   |
| 9             | 1             | 0           | -0.826735   | -0.611131   | -1.995982   |
| 10            | 1             | 0           | -1.705023   | 1.659911    | -1.531186   |
| 11            | 6             | 0           | -0.331677   | 3.712683    | -0.477384   |
| 12            | 6             | 0           | -0.762352   | 4.793911    | -0.147314   |
| 13            | 6             | 0           | -1.200893   | 6.092012    | 0.251065    |
| 14            | 6             | 0           | -0.248772   | 7.081210    | 0.531165    |
| 15            | 6             | 0           | -2.572886   | 6.407397    | 0.372011    |
| 16            | 6             | 0           | -0.635226   | 8.354534    | 0.918839    |
| 17            | 6             | 0           | -1.987815   | 8.666556    | 1.033274    |
| 18            | 6             | 0           | -2.944278   | 7.701067    | 0.761066    |
| 19            | 6             | 0           | -3.595857   | 5.446855    | 0.102734    |
| 20            | 6             | 0           | -4.520465   | 4.696247    | -0.107433   |
| 21            | 6             | 0           | -5.657876   | 3.885009    | -0.406813   |
| 22            | 6             | 0           | -6.781559   | 4.482383    | -0.992876   |
| 23            | 6             | 0           | -7.902109   | 3.732411    | -1.313749   |
| 24            | 6             | 0           | -7.918293   | 2.363776    | -1.055018   |
| 25            | 6             | 0           | -6.818301   | 1.756076    | -0.470542   |
| 26            | 6             | 0           | -5.679047   | 2.499365    | -0.132954   |
| 27            | 6             | 0           | -4.573690   | 1.836456    | 0.478692    |
| 28            | 6             | 0           | -3.678102   | 1.210098    | 0.997144    |
| 29            | 6             | 0           | -2.624155   | 0.423906    | 1.553511    |
| 30            | 6             | 0           | -1.495830   | 1.017667    | 2.137867    |
| 31            | 6             | 0           | -2.680226   | -0.972015   | 1.474061    |
| 32            | 6             | 0           | -0.443593   | 0.238872    | 2.585146    |
| 33            | 6             | 0           | -0.492954   | -1.150842   | 2.457444    |
| 34            | 6             | 0           | -1.630357   | -1.758053   | 1.924450    |
| 35            | 8             | 0           | 1.540108    | -1.431915   | -1.612504   |
| 36            | 8             | 0           | 0.612186    | -1.835568   | 2.877957    |
| 37            | 1             | 0           | 0.802735    | 6.832818    | 0.436992    |
| 38            | 1             | 0           | 0.119050    | 9.105237    | 1.130607    |
| 39            | 1             | 0           | -2.296721   | 9.661848    | 1.335147    |
| 40            | 1             | 0           | -3.999597   | 7.935074    | 0.849388    |
| 41            | 1             | 0           | -6.758188   | 5.547317    | -1.196952   |
| 42            | 1             | 0           | -8.761282   | 4.214069    | -1.768717   |
| 43            | 1             | 0           | -8.790607   | 1.770015    | -1.307915   |
| 44            | 1             | 0           | -6.823258   | 0.690313    | -0.268466   |
| 45            | 1             | 0           | -1.436899   | 2.098446    | 2.206305    |
| 46            | 1             | 0           | -3.550034   | -1.446938   | 1.032654    |
| 47            | 1             | 0           | 0.444943    | 0.692226    | 3.011283    |
| 48            | 1             | 0           | -1.701172   | -2.834850   | 1.833884    |
| 49            | 6             | 0           | 0.868703    | -3.122692   | 2.318926    |
|   |   |   | 2.672697 | -1.969394 | -0.932534 |
|---|---|---|----------|-----------|-----------|
| 51| 1 | 0 | 0.032745 | -3.806470 | 2.485466  |
| 52| 1 | 0 | 1.733996 | -3.507984 | -1.388354 |
| 53| 1 | 0 | 2.851625 | -2.944049 | -1.088987 |
| 54| 1 | 0 | 3.564024 | -3.037822 | 0.826921  |
| 55| 6 | 0 | 1.192265 | -3.037822 | 0.826921  |
| 56| 6 | 0 | 2.403639 | -2.143909 | 0.561847  |
| 57| 1 | 0 | 0.338333 | -2.601684 | 0.299308  |
| 58| 1 | 0 | 2.192835 | -1.165049 | 1.004476  |
| 59| 8 | 0 | 3.565920 | -2.706781 | 1.150174  |
| 60| 6 | 0 | 4.819547 | -0.632040 | 1.626673  |
| 61| 6 | 0 | 5.859153 | -0.660531 | 0.675174  |
| 62| 6 | 0 | 4.376415 | 0.594184  | 2.115344  |
| 63| 6 | 0 | 4.932584 | 1.793403  | 1.690565  |
| 64| 6 | 0 | 5.962607 | 1.801293  | 0.750017  |
| 65| 6 | 0 | 6.434704 | 0.562747  | 0.236291  |
| 66| 6 | 0 | 6.372417 | -1.891009 | 0.127011  |
| 67| 6 | 0 | 7.495709 | 0.556007  | -0.720652 |
| 68| 6 | 0 | 7.980959 | -0.673088 | -1.236422 |
| 69| 6 | 0 | 7.379794 | -1.893927 | -0.776343 |
| 70| 6 | 0 | 6.563722 | 3.024463  | 0.286750  |
| 71| 6 | 0 | 7.565098 | 3.014175  | -0.620548 |
| 72| 6 | 0 | 8.070590 | 1.778691  | -1.158739 |
| 73| 6 | 0 | 9.106877 | 1.747699  | -2.094950 |
| 74| 6 | 0 | 9.575753 | 0.539039  | -2.596023 |
| 75| 6 | 0 | 9.020016 | -0.660329 | -2.172290 |
| 76| 1 | 0 | 3.575759 | 0.609348  | 2.849715  |
| 77| 1 | 0 | 4.567740 | -2.555629 | 2.594466  |
| 78| 1 | 0 | 5.919093 | -2.825314 | 0.434364  |
| 79| 1 | 0 | 7.751973 | -2.832435 | -1.177159 |
| 80| 1 | 0 | 6.190602 | 3.962242  | 0.687926  |
| 81| 1 | 0 | 8.010878 | 3.943925  | -0.961853 |
| 82| 1 | 0 | 9.545603 | 2.683366  | -2.429331 |
| 83| 1 | 0 | 10.381704| 0.533371  | -3.322971 |
| 84| 1 | 0 | 9.388874 | -1.602958 | -2.566162 |
| 85| 6 | 0 | 4.191126 | -1.903888 | 2.148788  |
| 86| 1 | 0 | 3.465752 | -1.650813 | 2.931249  |
| 87| 1 | 0 | 4.947928 | -2.555629 | 2.594466  |
| 88| 8 | 0 | 1.432365 | -4.358512 | 0.363832  |
| 89| 6 | 0 | -0.859851| -4.948865 | -0.262877 |
| 90| 6 | 0 | -1.099276| -5.801922 | 0.817157  |
| 91| 6 | 0 | -1.940506| -4.276491 | -0.864412 |
| 92| 6 | 0 | -3.255425| -4.472006 | -0.343041 |
| 93| 6 | 0 | -3.467350| -5.338519 | 0.760466  |
| 94| 6 | 0 | -2.371089| -5.998190 | 1.323518  |
| 95| 6 | 0 | -1.794752| -3.840696 | -1.990511 |
| 96| 6 | 0 | -2.854454| -2.743578 | -2.534118 |
| 97| 6 | 0 | -4.184559| -2.912811 | -2.018688 |
| 98| 6 | 0 | -4.372042| -3.786748 | -0.916937 |
| 99| 6 | 0 | -4.799462| -5.141616 | 1.272514  |
|100| 6 | 0 | -5.851788| -4.863059 | 0.728891  |
|101| 6 | 0 | -5.676766| -3.971891 | -0.385406 |
|102| 6 | 0 | -6.751487| -3.284172 | -0.957573 |
|103| 6 | 0 | -6.556087| -2.429436 | -2.034422 |
|104| 6 | 0 | -5.284333| -2.245333 | -2.562797 |
105          6           0        0.582343   -4.787729   -0.697875
106          1           0       -2.526930   -6.667241   2.164658
107          1           0       -0.811848   -3.212364   -2.411150
108          1           0       -2.712812   -2.078664   -3.381496
109          1           0       -4.939246   -6.185133   2.114971
110          1           0       -6.853127   -5.000688   1.126199
111          1           0       -7.747315   -3.427591   -0.548344
112          1           0       -7.401548   -1.904232   -2.467388
113          1           0       -5.134065   -1.577000   -3.405518
114          1           0       -0.988227   -5.756701   -1.001348
115          1           0       -0.681674   -4.109768   -1.548163
116          1           0       -0.255189   -6.311063   1.271873

SCF Done:  E(RCAM-B3LYP) =  -2916.94694319

Full mass-weighted force constant matrix:
  Low frequencies ---   -3.8936   -0.0012   -0.0010    0.0013    2.4170
                    2.8724
  Low frequencies ---    5.4661    8.0792   10.3066
$p-(P,S,S)-2$: conformer d

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X         | Y         | Z         |
|----------------|---------------|-------------|-------------------------|-----------|-----------|-----------|
| 1              | 6             | 0           | -1.371465               | 1.543537  | -0.893017 |
| 2              | 6             | 0           | -2.739903               | 1.615508  | -0.677502 |
| 3              | 6             | 0           | -0.823734               | 0.397549  | -1.470153 |
| 4              | 6             | 0           | -1.661461               | -0.650275 | -1.860331 |
| 5              | 6             | 0           | -3.024570               | -0.572766 | -1.641523 |
| 6              | 6             | 0           | -3.585995               | 0.558563  | -1.030681 |
| 7              | 1             | 0           | -0.746230               | 2.374238  | -0.590979 |
| 8              | 1             | 0           | -3.157821               | 2.501191  | -0.210748 |
| 9              | 1             | 0           | -1.217483               | -1.529999 | -2.313452 |
| 10             | 1             | 0           | -3.655666               | -1.402594 | -1.918580 |
| 11             | 6             | 0           | -4.981573               | 0.628052  | -0.735909 |
| 12             | 6             | 0           | -6.154120               | 0.705926  | -0.448833 |
| 13             | 6             | 0           | -7.527770               | 0.886674  | -0.106682 |
| 14             | 6             | 0           | -8.003350               | 2.180599  | 0.145345  |
| 15             | 6             | 0           | -8.423242               | -0.201963 | -0.015987 |
| 16             | 6             | 0           | -9.331145               | 2.401866  | 0.475144  |
| 17             | 6             | 0           | -10.215259              | 1.328811  | 0.558459  |
| 18             | 6             | 0           | -9.763049               | 0.041711  | 0.314267  |
| 19             | 6             | 0           | -8.007902               | -1.547949 | -0.254698 |
| 20             | 6             | 0           | -7.746470               | -2.714631 | -0.436646 |
| 21             | 6             | 0           | -7.544554               | -4.104695 | -0.697572 |
| 22             | 6             | 0           | -8.590624               | -4.842686 | -1.263343 |
| 23             | 6             | 0           | -8.444144               | -6.193038 | -1.542704 |
| 24             | 6             | 0           | -7.242494               | -6.834031 | -1.250748 |
| 25             | 6             | 0           | -6.198230               | -6.121375 | -0.683012 |
| 26             | 6             | 0           | -6.328053               | -4.755855 | -0.395837 |
| 27             | 6             | 0           | -5.228752               | -4.063519 | 0.194713  |
| 28             | 6             | 0           | -4.258324               | -3.544486 | 0.696709  |
| 29             | 6             | 0           | -3.084958               | -2.949798 | 1.252657  |
| 30             | 6             | 0           | -1.850658               | -3.600695 | 1.147814  |
| 31             | 6             | 0           | -3.130011               | -1.696979 | 1.881875  |
| 32             | 6             | 0           | -0.687417               | -3.015462 | 1.626701  |
| 33             | 6             | 0           | -0.743863               | -1.755381 | 2.222136  |
| 34             | 6             | 0           | -1.974091               | -1.109203 | 2.362269  |
| 35             | 8             | 0           | 0.508510                | 0.212761  | -1.697360 |
| 36             | 8             | 0           | 0.343269                | -1.086403 | 2.707957  |
| 37             | 1             | 0           | -7.310724               | 3.012141  | 0.074536  |
| 38             | 1             | 0           | -9.677770               | 3.412289  | 0.665460  |
| 39             | 1             | 0           | -11.256332              | 1.495289  | 0.814537  |
| 40             | 1             | 0           | -10.44121               | -0.799807 | 0.379460  |
| 41             | 1             | 0           | -9.522010               | -4.335295 | -1.493821 |
| 42             | 1             | 0           | -9.266162               | -6.745422 | -1.985728 |
| 43             | 1             | 0           | -7.120145               | -7.890811 | -1.464126 |
| 44             | 1             | 0           | -5.261271               | -6.615123 | -0.449519 |
| 45             | 1             | 0           | -1.801641               | -4.574675 | 0.672830  |
| 46             | 1             | 0           | -4.078014               | -1.177277 | 1.967224  |
| 47             | 1             | 0           | 0.252370                | -3.543895 | 1.523814  |
| 48             | 1             | 0           | -1.998638               | -0.132125 | 2.832473  |
| 49             | 6             | 0           | 1.632685                | -1.364512 | 2.166891  |
|   |   |   | 1.452243 | 0.966821 | -0.939397 |
|---|---|---|----------|----------|-----------|
| 50| 6 | 0 | 1.889788 | -2.423180 | 2.275417 |
| 51| 1 | 0 | 2.330703 | -0.784905 | -1.369681 |
| 52| 1 | 0 | 2.424881 | 0.726922  | -1.041231 |
| 53| 1 | 0 | 1.284593 | 2.042291  | -1.041231 |
| 54| 6 | 0 | 1.744082 | -0.923529 | 0.706526  |
| 55| 6 | 0 | 1.439682 | 0.563087  | 0.534994  |
| 56| 6 | 0 | 1.107958 | -1.476063 | 0.098788  |
| 57| 6 | 0 | 0.445521 | 0.748163  | 0.953393  |
| 58| 8 | 0 | 2.410686 | 1.343010  | 1.213125  |
| 59| 6 | 0 | 1.040778 | 3.322291  | 1.767588  |
| 60| 6 | 0 | 1.546213 | 4.311707  | 0.899951  |
| 61| 6 | 0 | -0.276348| 3.412066  | 2.210162  |
| 62| 6 | 0 | -1.108777| 4.452249  | 1.818840  |
| 63| 6 | 0 | -0.640912| 5.447692  | 0.961068  |
| 64| 6 | 0 | 0.700951 | 5.381028  | 0.496671  |
| 65| 6 | 0 | 2.899564 | 4.287775  | 0.403958  |
| 66| 6 | 0 | 1.195901 | 6.399882  | -0.374169 |
| 67| 6 | 0 | 2.534879 | 6.349472  | -0.839492 |
| 68| 6 | 0 | 3.365906 | 5.256318  | -0.417837 |
| 69| 6 | 0 | -1.474248| 6.541442  | 0.535200  |
| 70| 6 | 0 | -1.003396| 7.501524  | -0.290999 |
| 71| 6 | 0 | 0.351049 | 7.468413  | -0.776635 |
| 72| 6 | 0 | 0.856945 | 8.453636  | -1.627941 |
| 73| 6 | 0 | 2.170114 | 8.396411  | -2.079692 |
| 74| 6 | 0 | 3.002365 | 7.355810  | -1.690559 |
| 75| 6 | 0 | -0.658732| 5.347857  | -2.881291 |
| 76| 6 | 0 | -2.131755| 4.496994  | 1.180885  |
| 77| 6 | 0 | 3.540736 | 3.460501  | 0.682136  |
| 78| 6 | 0 | 4.389086 | 5.219360  | -0.780715 |
| 79| 6 | 0 | -2.497520| 6.576615  | 0.897555  |
| 80| 6 | 0 | -1.641997| 8.322090  | -0.604924 |
| 81| 6 | 0 | 0.209937 | 9.270257  | -1.934957 |
| 82| 6 | 0 | 2.546818 | 9.170512  | -2.740673 |
| 83| 6 | 0 | 4.028004 | 7.314067  | -2.045528 |
| 84| 6 | 0 | 1.904364 | 2.179659  | 2.250601  |
| 85| 6 | 0 | 1.335959 | 2.907363  | 2.970077  |
| 86| 6 | 0 | 2.794944 | 2.556317  | 2.761548  |
| 87| 6 | 0 | 3.057963 | -1.178103 | 0.241935  |
| 88| 6 | 0 | 4.593201 | -2.492032 | -1.040035 |
| 89| 6 | 0 | 4.756714 | -2.464479 | -2.421837 |
| 90| 6 | 0 | 5.725459 | -2.615423 | -0.212282 |
| 91| 6 | 0 | 7.012012 | -2.725615 | -0.805711 |
| 92| 6 | 0 | 7.152208 | -2.700025 | -2.219327 |
| 93| 6 | 0 | 6.010042 | -2.566284 | -3.008538 |
| 94| 6 | 0 | 5.634896 | -2.640453 | 1.225194  |
| 95| 6 | 0 | 6.734971 | -2.777197 | 2.000434  |
| 96| 6 | 0 | 8.047087 | -2.897186 | 1.427524  |
| 97| 6 | 0 | 8.173102 | -2.867043 | 0.014864  |
| 98| 6 | 0 | 8.467287 | -2.814203 | -2.793120 |
| 99| 6 | 0 | 9.563633 | -2.947231 | -2.014190 |
|100| 6 | 0 | 9.458428 | -2.979761 | -0.579196 |
|101| 6 | 0 | 10.579434| -3.119171 | 0.242866  |
|102| 6 | 0 | 10.447002| -3.147710 | 1.625964  |
|103| 6 | 0 | 9.194408 | -3.037673 | 2.214439  |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|105| 6 | 0 | 3.205260 | -2.406421 | -0.464746 |
|106| 1 | 0 | 6.108265 | -2.543612 | -4.089825 |
|107| 1 | 0 | 4.661888 | -2.521640 | 1.686046 |
|108| 1 | 0 | 6.643816 | -2.791904 | 3.082789 |
|109| 1 | 0 | 8.557463 | -2.791120 | -3.875272 |
|110| 1 | 0 | 10.550714| -3.033051 | -2.459264|
|111| 1 | 0 | 11.561721| -3.205555 | -0.212596|
|112| 1 | 0 | 11.328626| -3.256370 | 2.249697 |
|113| 1 | 0 | 9.094951 | -3.059316 | 3.295841 |
|114| 1 | 0 | 2.468943 | -2.454603 | -1.276463|
|115| 1 | 0 | 3.011618 | -3.254234 | 0.207586 |
|116| 1 | 0 | 3.879271 | -2.364756 | -3.054162|

SCF Done: E(RCAM-B3LYP) = -2916.94663061
Full mass-weighted force constant matrix:
Low frequencies --- -2.4946 -0.0015 0.0004 0.0017 0.6967
2.9706
Low frequencies --- 4.2698 7.5607 8.6264
$p-(P,S,S)$-2: conformer \( e \)

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 6             | 0           | 3.214770 | 0.009185 | -1.880971|
| 2             | 6             | 0           | 4.535460 | 0.399577 | -1.786564|
| 3             | 6             | 0           | 2.205622 | 0.804075 | -1.330161|
| 4             | 6             | 0           | 2.526362 | 2.026801 | -0.743021|
| 5             | 6             | 0           | 3.857167 | 2.415545 | -0.657489|
| 6             | 6             | 0           | 4.881412 | 1.603978 | -1.153241|
| 7             | 1             | 0           | 2.941686 | -0.931553| -2.345598|
| 8             | 1             | 0           | 5.317737 | -0.237190| -2.184985|
| 9             | 1             | 0           | 1.757359 | 2.672776 | -0.338376|
| 10            | 1             | 0           | 4.107891 | 3.358098 | -0.182504|
| 11            | 6             | 0           | 6.247085 | 1.989883 | -0.986923|
| 12            | 6             | 0           | 7.392204 | 2.332882 | -0.802766|
| 13            | 6             | 0           | 8.706690 | 2.854274 | -0.604389|
| 14            | 6             | 0           | 8.904979 | 4.237716 | -0.712607|
| 15            | 6             | 0           | 9.809217 | 2.026833 | -0.299545|
| 16            | 6             | 0           | 10.159071| 4.798287 | -0.530764|
| 17            | 6             | 0           | 11.248219| 3.981414 | -0.237030|
| 18            | 6             | 0           | 11.071580| 2.611945 | -0.123957|
| 19            | 6             | 0           | 9.702891 | 0.608143 | -0.159649|
| 20            | 6             | 0           | 9.760578 | -0.590984| -0.008266|
| 21            | 6             | 0           | 10.003258| -1.922569| 0.134263 |
| 22            | 6             | 0           | 11.316033| -2.453261| -0.041842|
| 23            | 6             | 0           | 11.624687| -3.798736| 0.075913 |
| 24            | 6             | 0           | 10.620315| -4.716134| 0.374949 |
| 25            | 6             | 0           | 9.317993 | -4.279143| 0.556880 |
| 26            | 6             | 0           | 8.986436 | -2.921833| 0.443990 |
| 27            | 6             | 0           | 7.628083 | -2.528768| 0.642491 |
| 28            | 6             | 0           | 6.455807 | -2.293889| 0.825681 |
| 29            | 6             | 0           | 5.060009 | -2.035898| 0.989972 |
| 30            | 6             | 0           | 4.115693 | -2.942148| 0.499402 |
| 31            | 6             | 0           | 4.603324 | -0.864992| 1.615941 |
| 32            | 6             | 0           | 2.754444 | -2.678332| 0.582664 |
| 33            | 6             | 0           | 2.321017 | -1.486472| 1.161472 |
| 34            | 6             | 0           | 3.252024 | -0.598323| 1.707734 |
| 35            | 8             | 0           | 0.945044 | 0.299883 | -1.402505|
| 36            | 8             | 0           | 1.019463 | -1.100165| 1.228911|
| 37            | 1             | 0           | 8.052891 | 4.866796 | -0.945733|
| 38            | 1             | 0           | 10.287840| 5.871925 | -0.620302|
| 39            | 1             | 0           | 12.234051| 4.411702 | -0.095056|
| 40            | 1             | 0           | 11.913640| 1.968910 | 0.107698 |
| 41            | 1             | 0           | 12.091556| -1.732615| -0.277301|
| 42            | 1             | 0           | 12.647335| -4.132085| -0.066371|
| 43            | 1             | 0           | 10.852708| -5.771874| 0.468264 |
| 44            | 1             | 0           | 8.531200 | -4.986946| 0.793744 |
| 45            | 1             | 0           | 4.453094 | -3.860288| 0.030286 |
| 46            | 1             | 0           | 5.322953 | -0.155909| 2.010366 |
| 47            | 1             | 0           | 2.049070 | -3.396163| 0.183198 |
| 48            | 1             | 0           | 2.892652 | 0.316278 | 2.165704 |
| 49            | 6             | 0           | 0.053700 | -1.844282| 0.499564 |
| Row | Labels | Value 1  | Value 2  | Value 3  |
|-----|--------|---------|---------|---------|
| 50  | 6      | 0       | -0.085240 | 0.945421 | -0.668615 |
| 51  | 1      | 0       | -0.135122 | -2.802070 | 0.996880  |
| 52  | 1      | 0       | 0.412079  | -2.045038 | 0.349344  |
| 53  | 1      | 0       | 0.250515  | 1.163659  | -0.668615 |
| 54  | 1      | 0       | -0.352884 | 1.889117  | -1.156460 |
| 55  | 6      | 0       | -1.248780 | -1.042632 | 0.456593  |
| 56  | 6      | 0       | -1.302548 | 0.018102  | -0.641978 |
| 57  | 1      | 0       | 0.412079  | -2.045038 | -0.514148 |
| 58  | 1      | 0       | 0.250515  | 1.163659  | 0.349344  |
| 59  | 1      | 0       | -0.352884 | 1.889117  | -1.156460 |
| 60  | 1      | 0       | -4.292001 | 2.113914  | -1.257427 |
| 61  | 6      | 0       | -4.315325 | 3.217061  | -0.381728 |
| 62  | 1      | 0       | -1.374171 | -0.494964 | -1.611254 |
| 63  | 8      | 0       | -2.474534 | 0.780700  | -0.404391 |
| 64  | 6      | 0       | -4.292001 | 2.113914  | -1.257427 |
| 65  | 6      | 0       | -5.466179 | 1.726552  | -1.897007 |
| 66  | 6      | 0       | -6.662891 | 2.400636  | -1.696691 |
| 67  | 6      | 0       | -6.722016 | 3.497410  | -0.837431 |
| 68  | 6      | 0       | -5.537199 | 3.913348  | -0.172603 |
| 69  | 6      | 0       | -3.141409 | 3.682942  | 0.311517  |
| 70  | 6      | 0       | -5.581365 | 5.043871  | 0.700308  |
| 71  | 6      | 0       | -4.404644 | 5.478940  | 1.362298  |
| 72  | 6      | 0       | -7.944506 | 4.221419  | -0.608439 |
| 73  | 6      | 0       | -7.983531 | 5.286957  | 0.221707  |
| 74  | 6      | 0       | -8.840928 | 3.888111  | -1.123228 |
| 75  | 6      | 0       | -9.122239 | 5.825508  | 0.386672  |
| 76  | 6      | 0       | -7.754916 | 7.375805  | 1.919800  |
| 77  | 6      | 0       | -5.696196 | 8.122082  | 3.070649  |
| 78  | 6      | 0       | -3.563353 | 6.918160  | 2.717072  |
| 79  | 6      | 0       | -3.016371 | 1.376324  | -1.577141 |
| 80  | 6      | 0       | -2.288351 | 2.065121  | -2.025115 |
| 81  | 6      | 0       | -3.224915 | 0.595091  | -2.319236 |
| 82  | 6      | 0       | -2.316377 | -1.940547 | 0.212006  |
| 83  | 6      | 0       | -3.930345 | -3.501316 | 1.050362  |
| 84  | 6      | 0       | -3.696838 | -4.844881 | 1.328199  |
| 85  | 6      | 0       | -5.155745 | -3.115241 | 0.475447  |
| 86  | 6      | 0       | -6.143957 | -4.104509 | 0.220452  |
| 87  | 6      | 0       | -5.883279 | -5.469725 | 0.515157  |
| 88  | 6      | 0       | -4.649103 | -5.818615 | 1.063663  |
| 89  | 6      | 0       | -5.456775 | -1.745160 | 0.144277  |
| 90  | 6      | 0       | -6.661275 | -1.395413 | -0.363551 |
| 91  | 6      | 0       | -7.686137 | -2.370778 | -0.613695 |
| 92  | 6      | 0       | -7.410484 | -3.731745 | -0.325036 |
| 93  | 6      | 0       | -6.902242 | -6.449631 | 0.244534  |
| 94  | 6      | 0       | -8.098705 | -6.093679 | -0.273562 |
| 95  | 6      | 0       | -8.400351 | -4.719180 | -0.575125 |
| 96  | 6      | 0       | -9.634189 | -4.329065 | -1.101898 |
| 97  | 6      | 0       | -9.897150 | -2.993033 | -1.379992 |
| 98  | 6      | 0       | -8.934131 | -2.022292 | -1.139460 |
|   |   |   |      |      |      |
|---|---|---|------|------|------|
| 105| 6 | 0 | -2.880599 | -2.483118 | 1.400755 |
| 106| 1 | 0 | -4.441289 | -6.860105 | 1.290672 |
| 107| 1 | 0 | -4.686934 | -0.992714 | 0.276248 |
| 108| 1 | 0 | -6.869985 | -0.357170 | -0.603132 |
| 109| 1 | 0 | -6.685476 | -7.409520 | 0.471311 |
| 110| 1 | 0 | -8.860295 | -6.842594 | -0.470933 |
| 111| 1 | 0 | -10.390903 | -5.084751 | -1.292037 |
| 112| 1 | 0 | -10.861481 | -2.707265 | -1.788177 |
| 113| 1 | 0 | -9.142547 | -0.979160 | -1.359561 |
| 114| 1 | 0 | -2.103442 | -2.961002 | 2.010616 |
| 115| 1 | 0 | -3.308809 | -1.667260 | 1.999435 |
| 116| 1 | 0 | -2.747198 | -5.134099 | 1.769258 |

SCF Done: $E_{(RCA\text{M}-B3LYP)} = -2916.94601875$

Full mass-weighted force constant matrix:

Low frequencies ---  
-0.0025  -0.0015  0.0024  0.9773  1.9932  2.7438

Low frequencies ---  
6.3546  7.4153  8.6296
\textit{p-(P,S,S)-2: conformer f} \\

\textbf{Standard orientation:}

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X  | Y  | Z       |
| 1             | 6             | 0           | -0.306697 | -0.638727 | 1.764319 |
| 2             | 6             | 0           | -1.285339 | -1.593694 | 2.001675 |
| 3             | 6             | 0           | -0.665084 | 0.595446  | 1.221688 |
| 4             | 6             | 0           | -2.008547 | 0.872008  | 0.953129 |
| 5             | 6             | 0           | -2.977784 | -0.084728 | 1.188877 |
| 6             | 6             | 0           | -2.629329 | -1.342155 | 1.705562 |
| 7             | 1             | 0           | 0.725656  | -0.868340 | 1.997886 |
| 8             | 1             | 0           | -1.002504 | -2.557612 | 2.411165 |
| 9             | 1             | 0           | -2.263488 | 1.840696  | 0.536512 |
| 10            | 1             | 0           | -4.015076 | 0.124342  | 0.950615 |
| 11            | 6             | 0           | -3.609621 | -2.363265 | 1.894014 |
| 12            | 6             | 0           | -4.416166 | -3.253418 | 2.037008 |
| 13            | 6             | 0           | -5.310104 | -4.342234 | 2.264647 |
| 14            | 6             | 0           | -4.908573 | -5.389952 | 3.104323 |
| 15            | 6             | 0           | -6.590183 | -4.393411 | 1.669641 |
| 16            | 6             | 0           | -5.747697 | -6.463218 | 3.358526 |
| 17            | 6             | 0           | -7.012445 | -6.510205 | 2.776944 |
| 18            | 6             | 0           | -7.426461 | -5.484258 | 1.942242 |
| 19            | 6             | 0           | -7.064808 | -3.364559 | 0.799176 |
| 20            | 6             | 0           | -7.549750 | -2.546431 | 0.052012 |
| 21            | 6             | 0           | -8.225942 | -1.603220 | -0.781413 |
| 22            | 6             | 0           | -9.613057 | -1.457661 | -0.646014 |
| 23            | 6             | 0           | -10.316031| 0.555001  | -1.428149 |
| 24            | 6             | 0           | -9.640989 | 0.222197  | -2.366376 |
| 25            | 6             | 0           | -8.269824 | 0.088981  | -2.517537 |
| 26            | 6             | 0           | -7.542013 | -0.819286 | -1.736948 |
| 27            | 6             | 0           | -6.132300 | -0.927180 | -1.930441 |
| 28            | 6             | 0           | -4.943371 | -0.967208 | -2.149564 |
| 29            | 6             | 0           | -3.536090 | -0.972266 | -2.391486 |
| 30            | 6             | 0           | -2.719915 | -2.006969 | -1.910312 |
| 31            | 6             | 0           | -2.936010 | 0.083039  | -3.087080 |
| 32            | 6             | 0           | -1.350182 | -1.964669 | -2.092343 |
| 33            | 6             | 0           | -0.759241 | -0.885497 | -2.754089 |
| 34            | 6             | 0           | -1.561490 | 0.131240  | -3.272120 |
| 35            | 8             | 0           | 0.213311  | 1.595256  | 0.931319 |
| 36            | 8             | 0           | 0.600588  | -0.921957 | -2.855004 |
| 37            | 1             | 0           | -3.924288 | -5.344990 | 3.557501 |
| 38            | 1             | 0           | -5.416238 | -7.262978 | 4.012623 |
| 39            | 1             | 0           | -7.675081 | -7.346569 | 2.973262 |
| 40            | 1             | 0           | -8.408649 | -5.514104 | 1.483264 |
| 41            | 1             | 0           | -10.130366| -2.065085 | 0.088604 |
| 42            | 1             | 0           | -11.389567| -0.456800 | -1.305760 |
| 43            | 1             | 0           | -10.184308| 0.931466  | -2.982040 |
| 44            | 1             | 0           | -7.738844 | 0.688403  | -3.248954 |
| 45            | 1             | 0           | -3.169380 | -2.831274 | -1.367399 |
| 46            | 1             | 0           | -3.555456 | 0.883539  | -3.477289 |
| 47            | 1             | 0           | -0.710547 | -2.749850 | -1.704394 |
| 48            | 1             | 0           | -1.129358 | 0.963496  | -3.813789 |
| 49            | 6             | 0           | 1.326454  | 0.291548  | -3.035587 |
|   |   |   |          1.586821 |          1.291926 |          0.714352 |
|---|---|---|------------------|------------------|------------------|
|  50 | 6 | 0 |                  |                  |                  |
|  51 | 1 | 0 |          0.993242 |          0.825515 |          -3.931022 |
|  52 | 1 | 0 |          2.361800 |          -0.013842 |          -1.800329 |
|  53 | 1 | 0 |          2.080569 |          2.258351 |           0.617226 |
|  54 | 1 | 0 |          2.021657 |          0.770639 |          1.573595 |
|  55 | 6 | 0 |          1.250553 |          1.193443 |          -1.800329 |
|  56 | 6 | 0 |          1.797671 |          0.483085 |          -0.566989 |
|  57 | 1 | 0 |          0.208546 |          1.455785 |          -1.587305 |
|  58 | 1 | 0 |          1.270803 |          -0.475198 |          -0.491859 |
|  59 | 8 | 0 |          3.184739 |          0.260616 |          -0.741936 |
|  60 | 6 | 0 |          5.140136 |          -1.084355 |          -0.446651 |
|  61 | 6 | 0 |          5.820909 |          -2.256063 |          -0.066204 |
|  62 | 6 | 0 |          5.852342 |          -0.021135 |          -0.990415 |
|  63 | 6 | 0 |          7.227663 |          -0.092644 |          -1.166703 |
|  64 | 6 | 0 |          7.937822 |          -1.235797 |          -0.802038 |
|  65 | 6 | 0 |          7.228172 |          -2.332619 |          -0.244620 |
|  66 | 6 | 0 |          5.145620 |          -3.394395 |          0.503602 |
|  67 | 6 | 0 |          7.938603 |          -3.512520 |          0.135174 |
|  68 | 6 | 0 |          7.242130 |          -4.615549 |          0.693310 |
|  69 | 6 | 0 |          5.819495 |          -4.513996 |          0.862881 |
|  70 | 6 | 0 |          9.363252 |          -1.340181 |          -0.971641 |
|  71 | 6 | 0 |          10.033512 |         -2.457236 |          -0.611782 |
|  72 | 6 | 0 |          9.346041 |          -3.587328 |          -0.044122 |
|  73 | 6 | 0 |          10.019652 |          -4.751300 |          0.334360 |
|  74 | 6 | 0 |          9.329419 |          -5.827062 |          0.880268 |
|  75 | 6 | 0 |          7.954324 |          -5.762136 |          1.058997 |
|  76 | 1 | 0 |          5.312428 |          0.872311 |          -1.277886 |
|  77 | 1 | 0 |          7.762157 |          0.751032 |          -1.593966 |
|  78 | 1 | 0 |          4.071409 |          -3.355963 |          0.647572 |
|  79 | 1 | 0 |          5.288943 |          -5.357436 |          1.290204 |
|  80 | 1 | 0 |          9.891256 |          -0.492665 |          -1.399286 |
|  81 | 1 | 0 |          11.109457 |         -2.523855 |          -0.744686 |
|  82 | 1 | 0 |          11.095631 |         -4.807543 |          0.196641 |
|  83 | 1 | 0 |          9.869360 |          -6.723435 |          1.168623 |
|  84 | 1 | 0 |          7.418051 |          -6.604674 |          1.486009 |
|  85 | 6 | 0 |          3.644914 |          -0.986019 |          -0.262716 |
|  86 | 1 | 0 |          3.390892 |          -1.104785 |          0.801386 |
|  87 | 1 | 0 |          3.138774 |          -1.798705 |          -0.804517 |
|  88 | 8 | 0 |          2.013192 |          2.362677 |          -2.044148 |
|  89 | 6 | 0 |          0.382840 |          4.153862 |          -1.610918 |
|  90 | 6 | 0 |          -0.996033 |          4.132195 |          -1.799053 |
|  91 | 6 | 0 |          0.917239 |          4.841432 |          -0.503590 |
|  92 | 6 | 0 |          0.038443 |          5.503004 |          0.395430 |
|  93 | 6 | 0 |          -1.366163 |          5.462131 |          0.183283 |
|  94 | 6 | 0 |          -1.862341 |          4.770321 |          -0.921498 |
|  95 | 6 | 0 |          2.333517 |          4.909301 |          -0.245090 |
|  96 | 6 | 0 |          2.825698 |          5.588301 |          0.817228 |
|  97 | 6 | 0 |          1.960528 |          6.270168 |          1.738924 |
|  98 | 6 | 0 |          0.560466 |          6.217952 |          1.516800 |
|  99 | 6 | 0 |          -2.233004 |          6.141596 |          1.109872 |
| 100 | 6 | 0 |          -1.735804 |          6.816248 |          2.169949 |
| 101 | 6 | 0 |          -0.318844 |          6.881221 |          2.413700 |
| 102 | 6 | 0 |          0.214474 |          7.575850 |          3.502033 |
| 103 | 6 | 0 |          1.587631 |          7.622264 |          3.712004 |
| 104 | 6 | 0 |          2.453773 |          6.976407 |          2.840536 |
|    |    |    | 1.280841 | 3.452597 | -2.601902 |
|----|----|----|----------|----------|-----------|
|105 | 6  | 0  | -2.934155| 4.738299 | -1.093916 |
|106 | 1  | 0  | 3.010867 | 4.385221 | -0.908612 |
|107 | 1  | 0  | 3.896862 | 5.626379 | 0.993567  |
|108 | 1  | 0  | -3.304000| 6.099177 | 0.934401  |
|109 | 1  | 0  | -2.400339| 7.325726 | 2.861738  |
|110 | 1  | 0  | -0.458927| 8.082696 | 4.187143  |
|111 | 1  | 0  | 1.984607 | 8.166757 | 4.562884  |
|112 | 1  | 0  | 3.526318 | 7.014021 | 3.007801  |
|113 | 1  | 0  | 0.684280 | 3.114654 | -3.458148 |
|114 | 1  | 0  | 2.043236 | 4.133674 | -2.989001 |
|115 | 1  | 0  | -1.403224| 3.605904 | -2.657970 |

SCF Done:  \( E(\text{RCAM-B3LYP}) = -2916.94589383 \)

Full mass-weighted force constant matrix:

Low frequencies ---

\[ \begin{array}{cccccc}
    -2.5295 & -0.0016 & -0.0011 & 0.0013 & 2.9343 \\
    4.2630 & \\
\end{array} \]

Low frequencies ---

\[ \begin{array}{cccccc}
    6.7883 & 7.7520 & 8.8411 & \\
\end{array} \]
**p-(P,S,S)-2: conformer g**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -3.204311   | -0.384790   | -1.869648   |
| 2             | 6             | 0           | -4.545883   | -0.691685   | -1.764933   |
| 3             | 6             | 0           | -2.237210   | -1.306319   | -1.457547   |
| 4             | 6             | 0           | -2.626286   | -2.565624   | -1.003698   |
| 5             | 6             | 0           | -3.978508   | -2.868544   | -0.905879   |
| 6             | 6             | 0           | -4.957253   | -1.935522   | -1.259996   |
| 7             | 1             | 0           | -2.879199   | 0.583530    | -2.232918   |
| 8             | 1             | 0           | -5.292466   | 0.039867    | -2.054128   |
| 9             | 1             | 0           | -1.893340   | -3.307517   | -0.712372   |
| 10            | 1             | 0           | -4.281027   | -3.841216   | -0.532634   |
| 11            | 6             | 0           | -6.341226   | -2.241898   | -1.080210   |
| 12            | 6             | 0           | -7.502028   | -2.521522   | -0.887038   |
| 13            | 6             | 0           | -8.844954   | -2.965317   | -0.690391   |
| 14            | 6             | 0           | -9.153393   | -4.309501   | -0.941694   |
| 15            | 6             | 0           | -9.868956   | -2.099697   | -0.248164   |
| 16            | 6             | 0           | -10.439851  | -4.794218   | -0.768023   |
| 17            | 6             | 0           | -11.451534  | -3.938847   | -0.338305   |
| 18            | 6             | 0           | -11.165660  | -2.607553   | -0.082786   |
| 19            | 6             | 0           | -9.649744   | -0.717074   | 0.041578    |
| 20            | 6             | 0           | -9.611502   | 0.458788    | 0.324564    |
| 21            | 6             | 0           | -9.743652   | 1.849153    | 0.629591    |
| 22            | 6             | 0           | -11.025023  | 2.416027    | 0.569515    |
| 23            | 6             | 0           | -11.228133  | 3.758254    | 0.846251    |
| 24            | 6             | 0           | -10.146985  | 4.565559    | 1.191431    |
| 25            | 6             | 0           | -8.874177   | 4.022196    | 1.260612    |
| 26            | 6             | 0           | -8.648955   | 2.666004    | 0.986736    |
| 27            | 6             | 0           | -7.315934   | 2.161552    | 1.075610    |
| 28            | 6             | 0           | -6.156404   | 1.832693    | 1.176534    |
| 29            | 6             | 0           | -4.776546   | 1.468431    | 1.247802    |
| 30            | 6             | 0           | -3.792544   | 2.352867    | 0.797128    |
| 31            | 6             | 0           | -4.377269   | 0.216261    | 1.741803    |
| 32            | 6             | 0           | -2.450537   | 1.993993    | 0.792015    |
| 33            | 6             | 0           | -2.077722   | 0.728288    | 1.240934    |
| 34            | 6             | 0           | -3.045067   | -0.145152   | 1.746097    |
| 35            | 8             | 0           | -0.948133   | -0.881626   | -1.522507   |
| 36            | 8             | 0           | -0.804307   | 0.253742    | 1.216512    |
| 37            | 1             | 0           | -8.361202   | -4.968488   | -1.279803   |
| 38            | 1             | 0           | -10.654235  | -5.838579   | -0.969687   |
| 39            | 1             | 0           | -12.461988  | -4.309552   | -0.201417   |
| 40            | 1             | 0           | -11.946813  | -1.935316   | 0.255032    |
| 41            | 1             | 0           | -11.860864  | 1.781005    | 0.296855    |
| 42            | 1             | 0           | -12.228425  | 4.174900    | 0.791589    |
| 43            | 1             | 0           | -10.296481  | 5.618035    | 1.408811    |
| 44            | 1             | 0           | -8.027957   | 4.643464    | 1.532806    |
| 45            | 1             | 0           | -4.084347   | 3.330909    | 0.429460    |
| 46            | 1             | 0           | -5.127540   | -0.478131   | 2.103850    |
| 47            | 1             | 0           | -1.713902   | 2.697983    | 0.425553    |
| 48            | 1             | 0           | -2.731291   | -1.120112   | 2.101724    |
| 49            | 6             | 0           | 0.185348    | 0.994166    | 0.516880    |
|   |   |   | 0.064751 | -1.687520 | -0.936957 |
|---|---|---|----------|-----------|-----------|
| 50| 6 | 0  | 0.458456 | 1.885645  | 1.093085  |
| 51| 1 | 0  | -0.192666 | 1.312967  | -0.458772 |
| 52| 1 | 0  | -0.245870 | -2.031165 | 0.054359  |
| 53| 1 | 0  | 0.269197  | -2.559833 | -1.566351 |
| 54| 1 | 0  | 1.410094  | 0.092674  | 0.350505  |
| 55| 6 | 0  | 1.344078  | -0.857155 | -0.850029 |
| 56| 1 | 0  | 1.520306  | -0.515010 | 1.259433  |
| 57| 1 | 0  | 1.423741  | -0.259040 | -1.767076 |
| 58| 1 | 0  | 2.412249  | -1.785460 | -0.767294 |
| 59| 6 | 0  | 4.508087  | -2.644085 | -1.538789 |
| 60| 6 | 0  | 5.190988  | -2.939927 | -0.343751 |
| 61| 6 | 0  | 4.762434  | -3.407052 | 2.674603  |
| 62| 6 | 0  | 5.681229  | -4.447201 | -2.662796 |
| 63| 6 | 0  | 6.379750  | -4.762595 | -1.497439 |
| 64| 6 | 0  | 6.133616  | -4.002463 | -0.322805 |
| 65| 6 | 0  | 4.974239  | -2.197736 | 0.871496  |
| 66| 6 | 0  | 6.843165  | -4.311007 | 0.878496  |
| 67| 6 | 0  | 6.607978  | -3.558196 | 2.057872  |
| 68| 6 | 0  | 5.646144  | -2.491489 | 2.008594  |
| 69| 6 | 0  | 7.341554  | -5.832238 | -1.448157 |
| 70| 6 | 0  | 8.010897  | -6.122124 | -0.310379 |
| 71| 6 | 0  | 7.787539  | -5.371793 | 0.897425  |
| 72| 6 | 0  | 8.470259  | -5.655310 | 2.083010  |
| 73| 6 | 0  | 8.233312  | -4.913424 | 3.233953  |
| 74| 6 | 0  | 7.311681  | -3.875082 | 3.228325  |
| 75| 6 | 0  | 4.229888  | -3.177944 | -3.593142 |
| 76| 6 | 0  | 5.861242  | -5.024281 | -3.565044 |
| 77| 6 | 0  | 4.238261  | -1.403705 | 0.861401  |
| 78| 6 | 0  | 5.462569  | -1.923824 | 2.916943  |
| 79| 6 | 0  | 7.517809  | -6.404640 | -2.354296 |
| 80| 6 | 0  | 8.154260  | -6.931668 | -0.858999 |
| 81| 6 | 0  | 9.192392  | -6.466596 | 2.096361  |
| 82| 1 | 0  | 8.772339  | -5.147511 | 4.146541  |
| 83| 1 | 0  | 7.129081  | -3.297900 | 4.125689  |
| 84| 1 | 0  | 3.524332  | -1.506928 | -1.616601 |
| 85| 1 | 0  | 3.178701  | -1.395466 | -2.652833 |
| 86| 1 | 0  | 3.985629  | -0.560425 | -1.314809 |
| 87| 8 | 0  | 2.568357  | 0.889828  | 0.150195  |
| 88| 6 | 0  | 4.423597  | 2.140359  | 0.526701  |
| 89| 6 | 0  | 5.663921  | 1.618774  | 1.348875  |
| 90| 6 | 0  | 4.360590  | 3.379701  | 0.326701  |
| 91| 6 | 0  | 5.564352  | 4.082495  | 0.049807  |
| 92| 6 | 0  | 6.817730  | 3.531685  | 0.429562  |
| 93| 6 | 0  | 6.843726  | 2.295756  | 1.075042  |
| 94| 6 | 0  | 3.115900  | 3.975619  | -0.086290 |
| 95| 6 | 0  | 3.077828  | 5.176874  | -0.707097 |
| 96| 6 | 0  | 4.278181  | 5.913505  | -0.990544 |
| 97| 6 | 0  | 5.522655  | 5.350265  | -0.609786 |
| 98| 6 | 0  | 8.021058  | 4.265462  | 0.137791  |
| 99| 6 | 0  | 7.978156  | 5.464272  | -0.484563 |
| 100| 6 | 0 | 6.726246  | 6.053645  | -0.880342 |
| 101| 6 | 0 | 6.661075  | 7.293107  | -1.521707 |
| 102| 6 | 0 | 5.437527  | 7.837891  | -1.892457 |
| 103| 6 | 0 | 4.256692  | 7.156321  | -1.631049 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 105 | 6 | 0 | 3.175598 | 1.375020 | 1.343488 |
| 106 | 1 | 0 | 7.797433 | 1.864976 | 1.364994 |
| 107 | 1 | 0 | 2.195953 | 3.430947 | 0.086922 |
| 108 | 1 | 0 | 2.127459 | 5.606483 | -1.010895 |
| 109 | 1 | 0 | 8.970938 | 3.829165 | 0.432851 |
| 110 | 1 | 0 | 8.93182 | 6.008876 | -0.698721 |
| 111 | 1 | 0 | 7.582089 | 7.830298 | -1.728947 |
| 112 | 1 | 0 | 5.405357 | 8.801994 | -2.390009 |
| 113 | 1 | 0 | 3.302399 | 7.584643 | -1.923596 |
| 114 | 1 | 0 | 2.473074 | 2.013455 | 1.895797 |
| 115 | 1 | 0 | 3.428944 | 0.530708 | 1.997373 |
| 116 | 1 | 0 | 5.708857 | 0.656994 | 1.850788 |

SCF Done: E(RCAM-B3LYP) = -2916.94509319
Full mass-weighted force constant matrix:
Low frequencies --- -4.1177 -1.1338 -0.0024 -0.0015 0.0018 1.8471
Low frequencies --- 6.0462 7.0192 10.6384
**p-(P,S)-2:Ag : conformer a**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 6             | 0           | 0.207799    | 2.248150   | -0.907114  |
| 2             | 6             | 0           | -1.159052   | 2.420327   | -0.744343  |
| 3             | 6             | 0           | 0.680659    | 1.363982   | -1.880754  |
| 4             | 6             | 0           | -0.225703   | 0.685341   | -2.705644  |
| 5             | 6             | 0           | -1.583639   | 0.861314   | -2.540352  |
| 6             | 6             | 0           | -2.071707   | 1.725963   | -1.545842  |
| 7             | 1             | 0           | 0.885995    | 2.798745   | -0.267131  |
| 8             | 1             | 0           | -1.523389   | 3.099785   | 0.018637   |
| 9             | 1             | 0           | 0.163811    | 0.017197   | -3.465677  |
| 10            | 6             | 0           | -2.281014   | 0.326527   | -3.176145  |
| 11            | 6             | 0           | -3.481908   | 1.890574   | -1.362785  |
| 12            | 6             | 0           | -4.690789   | 2.046844   | -1.244833  |
| 13            | 6             | 0           | -6.035468   | 2.554332   | -1.345635  |
| 14            | 6             | 0           | -6.225952   | 3.809263   | -1.933695  |
| 15            | 6             | 0           | -7.157974   | 1.829562   | -0.888318  |
| 16            | 6             | 0           | -7.499538   | 4.341285   | -2.070366  |
| 17            | 6             | 0           | -8.606290   | 3.624698   | -1.623167  |
| 18            | 6             | 0           | -8.437124   | 2.379510   | -1.037662  |
| 19            | 6             | 0           | -7.037828   | 0.544143   | -0.271058  |
| 20            | 6             | 0           | -7.037705   | -0.545668  | 0.271126   |
| 21            | 6             | 0           | -7.157532   | -1.831121  | 0.888378   |
| 22            | 6             | 0           | -8.436556   | -2.381339  | 1.037819   |
| 23            | 6             | 0           | -8.605408   | -3.626589  | 1.623281   |
| 24            | 6             | 0           | -7.498466   | -4.342972  | 2.070334   |
| 25            | 6             | 0           | -6.225003   | -3.810682  | 1.933569   |
| 26            | 6             | 0           | -6.034834   | -2.555679  | 1.345561   |
| 27            | 6             | 0           | -4.690270   | -2.047894  | 1.244331   |
| 28            | 6             | 0           | -3.481426   | -1.891380  | 1.362705   |
| 29            | 6             | 0           | -2.071274   | -1.726466  | 1.545837   |
| 30            | 6             | 0           | -1.583448   | -0.861635  | 2.540307   |
| 31            | 6             | 0           | -1.158425   | -2.420703  | 0.744447   |
| 32            | 6             | 0           | -0.225559   | -0.885353  | 2.705661   |
| 33            | 6             | 0           | 0.680993    | -1.363863  | 1.880873   |
| 34            | 6             | 0           | 0.208379    | -2.248218  | 0.907282   |
| 35            | 8             | 0           | 1.986443    | 1.095065   | -2.112872  |
| 36            | 8             | 0           | 1.986709    | -1.094664  | 2.113044   |
| 37            | 1             | 0           | -5.360996   | 4.361359   | -2.283129  |
| 38            | 1             | 0           | -7.627470   | 5.315986   | -2.528310  |
| 39            | 1             | 0           | -9.603697   | 4.037081   | -1.729240  |
| 40            | 1             | 0           | -9.294988   | 1.817955   | -0.685850  |
| 41            | 1             | 0           | -9.294567   | -1.819945  | 0.686112   |
| 42            | 1             | 0           | -9.602721   | -4.039181  | 1.729433   |
| 43            | 1             | 0           | -7.626155   | -5.317724  | 2.528237   |
| 44            | 1             | 0           | -5.359900   | -4.362618  | 2.282892   |
| 45            | 1             | 0           | -2.280974   | -0.326945  | 3.176015   |
| 46            | 1             | 0           | -1.522570   | -3.100298  | -0.018501  |
| 47            | 1             | 0           | 0.163768    | -0.017060  | 3.465657   |
| 48            | 1             | 0           | 0.886735    | -2.798721  | 0.267389   |
| 49            | 6             | 0           | 2.990064    | -1.534659  | 1.198528   |
|     |   |   |          |          |          |
|-----|---|---|----------|----------|----------|
| 50  | 6 | 0 | 2.989677 | 1.535332 | -1.198355|
| 51  | 1 | 0 | 2.910026 | -2.608764|  1.011673|
| 52  | 1 | 0 | 3.936371 | -1.341441|  1.703049|
| 53  | 1 | 0 | 3.936043 |  1.342376| -1.702866|
| 54  | 1 | 0 | 2.909338 |  2.609414| -1.011501|
| 55  | 6 | 0 | 2.967380 | -0.755133| -0.117322|
| 56  | 6 | 0 | 2.967193 |  0.755795|  0.117496|
| 57  | 1 | 0 | 2.062247 | -0.998835| -0.682988|
| 58  | 1 | 0 | 2.061999 |  0.999272|  0.682965|
| 59  | 8 | 0 | 4.117478 |  1.135853|  0.851438|
| 60  | 6 | 0 | 3.276671 |  3.217289|  1.872148|
| 61  | 6 | 0 | 3.988579 |  4.227839|  1.193731|
| 62  | 6 | 0 | 2.015703 |  3.502445|  2.390974|
| 63  | 6 | 0 | 1.439000 |  4.759276|  2.258665|
| 64  | 6 | 0 | 2.118060 |  5.782646|  1.596974|
| 65  | 6 | 0 | 3.407205 |  5.518068|  1.059098|
| 66  | 6 | 0 | 5.296315 |  4.006417|  0.628732|
| 67  | 6 | 0 | 4.116124 |  6.559859|  0.385533|
| 68  | 6 | 0 | 5.404795 |  6.310726| -0.152791|
| 69  | 6 | 0 | 5.966202 |  4.996491| -0.006029|
| 70  | 6 | 0 | 1.554065 |  7.098535|  1.445899|
| 71  | 6 | 0 | 2.227491 |  8.081199|  0.807152|
| 72  | 6 | 0 | 3.535534 |  7.849561|  0.252678|
| 73  | 6 | 0 | 4.247838 |  8.853004| -0.409065|
| 74  | 6 | 0 | 5.510108 |  8.600316| -0.934009|
| 75  | 6 | 0 | 6.084556 |  7.342528| -0.808394|
| 76  | 1 | 0 | 1.475573 |  2.721719|  2.916393|
| 77  | 1 | 0 | 0.455802 |  4.954874|  2.676518|
| 78  | 1 | 0 | 5.734117 |  3.018261|  0.699210|
| 79  | 1 | 0 | 6.951056 |  4.809209| -0.424160|
| 80  | 1 | 0 | 0.568256 |  7.284112|  1.862184|
| 81  | 1 | 0 | 1.791873 |  9.070453|  0.701113|
| 82  | 1 | 0 | 3.803371 |  9.838861| -0.509776|
| 83  | 1 | 0 | 6.049546 |  9.391420| -1.444940|
| 84  | 1 | 0 | 7.070728 |  7.148479| -1.219981|
| 85  | 6 | 0 | 3.861275 |  1.837667|  2.066736|
| 86  | 1 | 0 | 3.194187 |  1.242570|  2.701083|
| 87  | 1 | 0 | 4.833247 |  1.893976|  2.564054|
| 88  | 8 | 0 | 4.117762 | -1.134904| -0.851263|
| 89  | 6 | 0 | 3.277474 | -3.216507| -1.872072|
| 90  | 6 | 0 | 2.016594 | -3.501963| -2.390948|
| 91  | 6 | 0 | 3.989625 | -4.226910| -1.193689|
| 92  | 6 | 0 | 3.408578 | -5.517295| -1.059141|
| 93  | 6 | 0 | 2.119518 | -5.782180| -1.597069|
| 94  | 6 | 0 | 1.440213 | -4.758952| -2.258726|
| 95  | 6 | 0 | 5.297293 | -4.005184| -0.628652|
| 96  | 6 | 0 | 5.967417 | -4.995121|  0.006073|
| 97  | 6 | 0 | 5.406341 | -6.309505|  0.152757|
| 98  | 6 | 0 | 4.117747 | -6.558940| -0.385611|
| 99  | 6 | 0 | 1.555857 | -7.098221| -1.446080|
|100  | 6 | 0 | 2.229515 | -8.080745| -0.807363|
|101  | 6 | 0 | 3.537483 | -7.848798| -0.252838|
|102  | 6 | 0 | 4.250026 | -8.852092|  0.408874|
|103  | 6 | 0 | 5.512217 | -8.599107|  0.933865|
|104  | 6 | 0 | 6.086347 | -7.341167|  0.808327|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 105 | 6 | 0 | 3.861732 | -1.836730 | -2.066592 |
| 106 | 1 | 0 | 0.457079 | -4.954783 | -2.676620 |
| 107 | 1 | 0 | 5.734847 | -3.016914 | -0.699074 |
| 108 | 1 | 0 | 6.952216 | -4.807611 | 0.424231  |
| 109 | 1 | 0 | 0.570108 | -7.284031 | -1.862405 |
| 110 | 1 | 0 | 1.794150 | -9.070116 | -0.701387 |
| 111 | 1 | 0 | 3.805806 | -9.838066 | 0.509526  |
| 112 | 1 | 0 | 6.051843 | -9.390100 | 1.444771  |
| 113 | 1 | 0 | 7.072459 | -7.146888 | 1.219948  |
| 114 | 1 | 0 | 4.833717 | -1.892772 | -2.563916 |
| 115 | 1 | 0 | 3.194493 | -1.241767 | -2.700904 |
| 116 | 1 | 0 | 1.476273 | -2.721348 | -2.919585 |
| 117 | 47 | 0 | -4.477795 | -0.000501 | -0.000042 |

SCF Done:  E(RCAM-B3LYP) = -3062.46810707

Full mass-weighted force constant matrix:

Low frequencies --- -1.6556  -0.0021  -0.0009  0.0016  3.1195
5.3876

Low frequencies ---  7.2567  7.3566  13.7481
$p$-$(P,S)-2:Ag$ : conformer $b$

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 2.523837    | 0.628958    | -1.746991   |
| 2             | 6             | 0           | 3.841673    | 1.030236    | -1.736267   |
| 3             | 6             | 0           | 1.634949    | 1.105878    | -0.775302   |
| 4             | 6             | 0           | 2.067022    | 2.038683    | 0.169004    |
| 5             | 6             | 0           | 3.398172    | 2.434809    | 0.179298    |
| 6             | 6             | 0           | 4.304828    | 1.924210    | -0.754705   |
| 7             | 1             | 0           | 2.158326    | -0.076531   | -0.080508   |
| 8             | 1             | 0           | 4.532709    | 0.643690    | -2.477812   |
| 9             | 1             | 0           | 1.385735    | 2.445183    | 0.905641    |
| 10            | 1             | 0           | 3.740471    | 3.138484    | 0.930333    |
| 11            | 6             | 0           | 5.694363    | 2.268166    | -0.693636   |
| 12            | 6             | 0           | 6.880831    | 2.564789    | -0.643920   |
| 13            | 6             | 0           | 8.166503    | 3.210090    | -0.695795   |
| 14            | 6             | 0           | 8.206417    | 4.590147    | -0.922136   |
| 15            | 6             | 0           | 9.379797    | 2.503172    | -0.532072   |
| 16            | 6             | 0           | 9.417496    | 5.262914    | -0.987243   |
| 17            | 6             | 0           | 10.612256   | 4.565705    | -0.830251   |
| 18            | 6             | 0           | 10.593447   | 3.197878    | -0.605350   |
| 19            | 6             | 0           | 9.421753    | 1.091637    | -0.290323   |
| 20            | 6             | 0           | 9.572032    | -0.099910   | -0.80508    |
| 21            | 6             | 0           | 9.876418    | -1.481404   | 0.145457    |
| 22            | 6             | 0           | 11.219304   | -1.876883   | 0.112000    |
| 23            | 6             | 0           | 11.570706   | -3.202763   | 0.313233    |
| 24            | 6             | 0           | 10.585188   | -4.156605   | 0.552401    |
| 25            | 6             | 0           | 9.250524    | -3.781764   | 0.594211    |
| 26            | 6             | 0           | 8.875823    | -2.448761   | 0.394210    |
| 27            | 6             | 0           | 7.477146    | -2.116450   | 0.457633    |
| 28            | 6             | 0           | 6.263143    | -2.091008   | 0.609151    |
| 29            | 6             | 0           | 4.842966    | -2.052194   | 0.794209    |
| 30            | 6             | 0           | 3.985821    | -2.760927   | -0.053364   |
| 31            | 6             | 0           | 4.289207    | -1.258910   | 1.814778    |
| 32            | 6             | 0           | 2.606906    | -2.658057   | 0.080680    |
| 33            | 6             | 0           | 2.072262    | -1.825084   | 1.065012    |
| 34            | 6             | 0           | 2.922773    | -1.149900   | 1.949531    |
| 35            | 8             | 0           | 0.386646    | 0.593036    | -0.832853   |
| 36            | 8             | 0           | 0.753715    | -1.594330   | 1.243856    |
| 37            | 1             | 0           | 7.273517    | 5.127796    | -1.047518   |
| 38            | 1             | 0           | 9.427813    | 6.332977    | -1.163062   |
| 39            | 1             | 0           | 11.561080   | 5.088251    | -0.882206   |
| 40            | 1             | 0           | 11.520578   | 2.650663    | -0.480968   |
| 41            | 1             | 0           | 11.982118   | -1.130223   | -0.077090   |
| 42            | 1             | 0           | 12.615405   | -3.492038   | 0.281836    |
| 43            | 1             | 0           | 10.855707   | -5.195031   | 0.709262    |
| 44            | 1             | 0           | 8.479740    | -4.519841   | 0.784426    |
| 45            | 1             | 0           | 4.401479    | -3.388585   | -0.834179   |
| 46            | 1             | 0           | 4.945089    | -0.718295   | 2.489236    |
| 47            | 1             | 0           | 1.963716    | -3.212251   | -0.591354   |
| 48            | 1             | 0           | 2.480335    | -0.526048   | 2.719220    |
| 49            | 6             | 0           | -0.192910   | -2.116107   | 0.317484    |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
| 50| 6 | 0 | -0.552143 | 0.895978 | 0.192572 |
| 51| 1 | 0 | -0.285234 | -3.199623 | -0.709227 |
| 52| 1 | 0 | -0.120860 | -1.909210 | 0.781945  |
| 53| 1 | 0 | -0.094692 | -1.909210 | 0.781945  |
| 54| 1 | 0 | -0.904432 | 1.927437  | 0.083506  |
| 55| 6 | 0 | -1.536756 | -1.454030 | 0.627238  |
| 56| 6 | 0 | -1.731941 | 0.062083  | 0.024103  |
| 57| 1 | 0 | -1.627230 | -1.362417 | 1.718449  |
| 58| 1 | 0 | -1.927115 | -0.187301 | -1.048859 |
| 59| 8 | 0 | -2.861510 | 0.493652  | 0.672609  |
| 60| 6 | 0 | -4.771543 | 1.938855  | 0.647751  |
| 61| 6 | 0 | -5.775382 | 2.687827  | 0.003056  |
| 62| 6 | 0 | -4.795452 | 1.807021  | 2.032366  |
| 63| 6 | 0 | -5.796605 | 2.394473  | 2.794803  |
| 64| 6 | 0 | -6.810436 | 3.138981  | 2.192860  |
| 65| 6 | 0 | -6.801308 | 3.290570  | 0.780133  |
| 66| 6 | 0 | -5.807948 | 2.873202  | -1.426001 |
| 67| 6 | 0 | -7.830317 | 4.053378  | 0.146574  |
| 68| 6 | 0 | -7.832299 | 4.215536  | -1.263183 |
| 69| 6 | 0 | -6.782476 | 3.597132  | -2.024391 |
| 70| 6 | 0 | -7.862480 | 3.758393  | 2.955562  |
| 71| 6 | 0 | -8.835421 | 4.478523  | 2.353893  |
| 72| 6 | 0 | -8.856050 | 4.654068  | 0.925032  |
| 73| 6 | 0 | -9.851697 | 5.395654  | 0.283669  |
| 74| 6 | 0 | -9.846126 | 5.548960  | -1.098097 |
| 75| 6 | 0 | -8.847286 | 4.965653  | -1.866054 |
| 76| 1 | 0 | -4.015492 | 1.231035  | 2.514216  |
| 77| 1 | 0 | -5.794414 | 2.274665  | 3.874355  |
| 78| 1 | 0 | -5.033565 | 2.422780  | -2.036895 |
| 79| 1 | 0 | -6.786735 | 3.723025  | -3.103209 |
| 80| 1 | 0 | -7.855218 | 3.631714  | 4.034280  |
| 81| 1 | 0 | -9.624180 | 4.940932  | 2.940173  |
| 82| 1 | 0 | -10.635477| 5.854540  | 0.879324  |
| 83| 1 | 0 | -10.627722| 6.128455  | -1.579073 |
| 84| 1 | 0 | -8.845888 | 5.087342  | -2.945347 |
| 85| 6 | 0 | -3.678782 | 1.287056  | -0.164714 |
| 86| 1 | 0 | -3.075592 | 2.057245  | -0.668522 |
| 87| 1 | 0 | -4.112351 | 0.652095  | -0.950016 |
| 88| 8 | 0 | -2.580219 | -3.910047 | 0.403925  |
| 89| 6 | 0 | -4.278861 | -3.910047 | 0.403925  |
| 90| 6 | 0 | -4.196010 | -5.265909 | 0.101150  |
| 91| 6 | 0 | -5.477006 | -3.214564 | 0.149512  |
| 92| 6 | 0 | -6.584020 | -3.917151 | -0.398900 |
| 93| 6 | 0 | -6.476213 | -5.302553 | -0.696908 |
| 94| 6 | 0 | -5.271024 | -5.957086 | -0.440467 |
| 95| 6 | 0 | -5.631294 | -1.809595 | 0.432908  |
| 96| 6 | 0 | -6.800532 | -1.168855 | 0.198712  |
| 97| 6 | 0 | -7.937303 | -1.854726 | -0.350444 |
| 98| 6 | 0 | -7.815196 | -3.236338 | -0.649427 |
| 99| 6 | 0 | -7.613960 | -5.988227 | -1.251910 |
|100| 6 | 0 | -8.776625 | -5.340617 | -1.489326 |
|101| 6 | 0 | -8.922369 | -3.938910 | -1.195732 |
|102| 6 | 0 | -10.116808| -3.252472 | -1.430469 |
|103| 6 | 0 | -10.227710| -1.898383 | -1.135974 |
|104| 6 | 0 | -9.149956 | -1.204467 | -0.601698 |
|   |   |   |   |   |
|---|---|---|---|---|
| 105 | 6 | 0 | -3.095321 | -3.215272 | 1.020632 |
| 106 | 1 | 0 | -5.180384 | -7.015445 | -0.666315 |
| 107 | 1 | 0 | -4.782009 | -1.256482 | 0.816655 |
| 108 | 1 | 0 | -6.895449 | -0.109757 | 0.420437 |
| 109 | 1 | 0 | -7.514689 | -7.046367 | -1.475936 |
| 110 | 1 | 0 | -9.628023 | -5.869544 | -1.907763 |
| 111 | 1 | 0 | -10.963097 | -3.790732 | -1.847502 |
| 112 | 1 | 0 | -11.162757 | -1.380580 | -1.324826 |
| 113 | 1 | 0 | -9.239331 | -0.146286 | -0.373611 |
| 114 | 1 | 0 | -2.326555 | -3.956287 | 1.275467 |
| 115 | 1 | 0 | -3.382652 | -2.707586 | 1.951975 |
| 116 | 1 | 0 | -3.267588 | -5.794082 | 0.298637 |
| 117 | 47 | 0 | 7.026031 | 0.211835 | -0.085135 |

SCF Done: E(RCAM-B3LYP) = -3062.46674574

Full mass-weighted force constant matrix:

Low frequencies --- -1.3558 -0.0130 -0.0007 0.0025 3.1277

5.2531

Low frequencies --- 7.0117 7.3042 13.5223
\( p-(P,S)-2:Ag \) : conformer e

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 6             | 0           | 1.781969   | -0.835175  | 0.816659   |
| 2             | 6             | 0           | 0.855056   | -1.865269  | 0.878868   |
| 3             | 6             | 0           | 1.478230   | 0.401032   | 1.392717   |
| 4             | 6             | 0           | 0.252923   | 0.586533   | 2.045018   |
| 5             | 6             | 0           | -0.664473  | -0.441866  | 2.104504   |
| 6             | 6             | 0           | -0.378583  | -1.683943  | 1.513535   |
| 7             | 1             | 0           | 2.725292   | -1.006892  | 0.313700   |
| 8             | 1             | 0           | 1.091028   | -2.822243  | 0.426029   |
| 9             | 1             | 0           | 0.036934   | 1.554068   | 2.484407   |
| 10            | 1             | 0           | -1.615145  | -0.291329  | 2.604763   |
| 11            | 6             | 0           | -1.335857  | -2.746889  | 1.570815   |
| 12            | 6             | 0           | -2.148628  | -3.658108  | 1.663401   |
| 13            | 6             | 0           | -2.876635  | -4.827675  | 2.084347   |
| 14            | 6             | 0           | -2.302890  | -5.648993  | 3.060581   |
| 15            | 6             | 0           | -4.144253  | -5.162497  | 1.559469   |
| 16            | 6             | 0           | -2.966580  | -6.779420  | 3.513837   |
| 17            | 6             | 0           | -4.218537  | -7.106378  | 2.999928   |
| 18            | 6             | 0           | -4.802664  | -6.304652  | 2.031406   |
| 19            | 6             | 0           | -4.786738  | -4.373175  | 0.553552   |
| 20            | 6             | 0           | -5.408968  | -3.772912  | -0.303338  |
| 21            | 6             | 0           | -6.238947  | -3.135656  | -1.279640  |
| 22            | 6             | 0           | -7.552474  | -3.594521  | -1.437995  |
| 23            | 6             | 0           | -8.398562  | -3.006966  | -2.365764  |
| 24            | 6             | 0           | -7.945829  | -1.951029  | -3.152158  |
| 25            | 6             | 0           | -6.646471  | -1.486967  | -3.010731  |
| 26            | 6             | 0           | -5.778152  | -2.067235  | -2.079993  |
| 27            | 6             | 0           | -4.436225  | -1.551424  | -1.987990  |
| 28            | 6             | 0           | -3.393931  | -0.941243  | -2.189748  |
| 29            | 6             | 0           | -2.187606  | -0.224550  | -2.474565  |
| 30            | 6             | 0           | -1.157934  | -0.835410  | -3.210106  |
| 31            | 6             | 0           | -2.014679  | 1.090466   | -2.029198  |
| 32            | 6             | 0           | 0.013027   | -0.153633  | -3.467393  |
| 33            | 6             | 0           | 0.188811   | 1.152936   | -2.994201  |
| 34            | 6             | 0           | -0.839139  | 1.781394   | -2.286330  |
| 35            | 8             | 0           | 2.299145   | 1.478889   | 1.382888   |
| 36            | 8             | 0           | 1.386835   | 1.714083   | -3.281807  |
| 37            | 1             | 0           | -1.329528  | -5.387636  | 3.459746   |
| 38            | 1             | 0           | -2.505802  | -7.404610  | 4.270763   |
| 39            | 1             | 0           | -4.740759  | -7.988763  | 3.353164   |
| 40            | 1             | 0           | -5.776245  | -6.555109  | 1.625789   |
| 41            | 1             | 0           | -7.900327  | -4.156216  | -0.821719  |
| 42            | 1             | 0           | -9.413588  | -3.373123  | -2.474164  |
| 43            | 1             | 0           | -8.604818  | -1.488099  | -3.878496  |
| 44            | 1             | 0           | -6.287353  | -0.667210  | -3.622355  |
| 45            | 1             | 0           | -1.285325  | -1.849985  | -3.571891  |
| 46            | 1             | 0           | -2.807452  | 1.576150   | -1.470649  |
| 47            | 1             | 0           | 0.816551   | -0.614036  | -4.031353  |
| 48            | 1             | 0           | -0.736087  | 2.797849   | -1.927409  |
| 49            | 6             | 0           | 1.769027   | 2.951465   | -2.685685  |
|   |   |   | 3.442376 | 1.508254 | 0.529963 |
|---|---|---|----------|----------|----------|
| 50| 6 | 0 | 0.999201 | 3.712485 | -2.836420 |
| 51| 1 | 0 | 2.668285 | 3.257379 | -3.220170 |
| 52| 1 | 0 | 4.009875 | 2.385506 | 0.841257  |
| 53| 1 | 0 | 4.070858 | 0.626672 | 0.680705  |
| 54| 6 | 0 | 2.107083 | 2.817665 | -1.199249 |
| 55| 6 | 0 | 3.070152 | 1.653732 | -0.946218 |
| 56| 1 | 0 | 1.194923 | 2.630878 | -0.522963 |
| 57| 1 | 0 | 2.575317 | 0.740664 | -1.292402 |
| 58| 8 | 0 | 2.668285 | 3.257379 | -3.220170 |
| 59| 6 | 0 | 4.954665 | -0.502569 | -1.954114 |
| 60| 6 | 0 | 6.039892 | -0.655153 | -1.078013 |
| 61| 6 | 0 | 4.158451 | -1.610388 | -2.260264 |
| 62| 6 | 0 | 4.424734 | -2.865439 | -1.728217 |
| 63| 6 | 0 | 5.503461 | -3.052336 | -0.863443 |
| 64| 6 | 0 | 6.322281 | -1.937725 | -0.533712 |
| 65| 6 | 0 | 6.895892 | 0.445412 | -0.711430 |
| 66| 6 | 0 | 7.434342 | -2.116999 | 0.345287  |
| 67| 6 | 0 | 8.261961 | -1.014287 | 0.679795  |
| 68| 6 | 0 | 7.949838 | 0.271462 | 0.119789  |
| 69| 6 | 0 | 5.814051 | -4.339593 | -0.298632 |
| 70| 6 | 0 | 6.866415 | -4.504793 | 0.533411  |
| 71| 6 | 0 | 7.717861 | -3.399288 | 0.886783  |
| 72| 6 | 0 | 8.811476 | -3.551317 | 1.742897  |
| 73| 6 | 0 | 9.617430 | -2.465536 | 2.065694  |
| 74| 6 | 0 | 9.347035 | -1.208881 | 1.540788  |
| 75| 6 | 0 | 3.319368 | -1.487306 | -2.939429 |
| 76| 6 | 0 | 3.796294 | -3.712054 | -1.988504 |
| 77| 6 | 0 | 6.668997 | 1.432087 | 1.096371  |
| 78| 6 | 0 | 8.582729 | 1.113948 | 0.383587  |
| 79| 6 | 0 | 5.179127 | -5.180949 | -0.560714 |
| 80| 6 | 0 | 7.091650 | -5.481353 | 0.951953  |
| 81| 6 | 0 | 9.027796 | -4.532399 | 2.155607  |
| 82| 6 | 0 | 10.463418 | -2.601500 | 2.731792  |
| 83| 6 | 0 | 9.979137 | -0.363174 | 1.795224  |
| 84| 6 | 0 | 4.621203 | 0.830064 | -2.588514 |
| 85| 6 | 0 | 3.807301 | 0.701159 | -3.310744 |
| 86| 6 | 0 | 5.487073 | 1.225027 | -3.126610 |
| 87| 6 | 0 | 2.679888 | 4.057478 | -0.817065 |
| 88| 6 | 0 | 0.752218 | 5.218711 | 0.156488  |
| 89| 6 | 0 | 0.486541 | 5.862400 | -1.052441 |
| 90| 6 | 0 | -0.251050 | 5.160258 | 1.142994  |
| 91| 6 | 0 | -1.525802 | 5.739793 | 0.872513  |
| 92| 6 | 0 | -1.774878 | 6.373361 | -0.373264 |
| 93| 6 | 0 | -0.749699 | 6.426658 | -1.320515 |
| 94| 6 | 0 | -0.054528 | 4.546638 | 2.435373  |
| 95| 6 | 0 | -1.041072 | 4.502319 | 3.360511  |
| 96| 6 | 0 | -2.336964 | 5.068223 | 3.107053  |
| 97| 6 | 0 | -2.566364 | 5.689205 | 1.851990  |
| 98| 6 | 0 | -3.069892 | 6.947269 | -0.624152 |
| 99| 6 | 0 | -4.052412 | 6.894821 | 0.302925  |
|100| 6 | 0 | -3.836743 | 6.263806 | 1.577330  |
|101| 6 | 0 | -4.388853 | 6.202145 | 2.550463  |
|102| 6 | 0 | -4.604286 | 5.590315 | 3.775417  |
|103| 6 | 0 | -3.364614 | 5.028541 | 4.053625  |
|   |   |   |       |       |       |
|---|---|---|-------|-------|-------|
|105| 6 | 0 | 2.137877 | 4.638600 | 0.364161 |
|106| 1 | 0 | -0.928417 | 6.920367 | -2.271275 |
|107| 1 | 0 | 0.909677  | 4.119198 | 2.681803  |
|108| 1 | 0 | -0.862291 | 4.038588 | 4.326398  |
|109| 1 | 0 | -3.239209 | 7.428376 | -1.583019 |
|110| 1 | 0 | -5.026169 | 7.332277 | 0.103089  |
|111| 1 | 0 | -5.808701 | 6.642349 | 2.337692  |
|112| 1 | 0 | -5.393254 | 5.553332 | 4.519788  |
|113| 1 | 0 | -3.182336 | 4.554129 | 5.013535  |
|114| 1 | 0 | 2.841616  | 5.431762 | 0.635219  |
|115| 1 | 0 | 2.142542  | 3.901804 | 1.168769  |
|116| 1 | 0 | 1.275897  | 5.915546 | -1.794672 |
|117| 47| 0 | -3.121816 | -2.485082| -0.196127 |

SCF Done:  \( E(\text{RCAM-B3LYP}) = -3062.46565018 \)

Full mass-weighted force constant matrix:

Low frequencies --- -2.0948 -0.0010 -0.0006 0.0012 2.9289 3.6445

Low frequencies --- 6.6204 7.4160 8.5387
**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 0.654202    | 1.489209    | 0.884788    |
| 2             | 6             | 0           | 2.038230    | 1.473987    | 0.971701    |
| 3             | 6             | 0           | -0.093644   | 0.577307    | 1.634777    |
| 4             | 6             | 0           | 0.556049    | -0.320872   | 2.490890    |
| 5             | 6             | 0           | 1.932909    | -0.330947   | 2.574458    |
| 6             | 6             | 0           | 2.696607    | 0.562096    | 1.804199    |
| 7             | 1             | 0           | 0.176755    | 2.205205    | 0.227791    |
| 8             | 1             | 0           | 2.616854    | 2.176293    | 0.381382    |
| 9             | 1             | 0           | -0.045197   | -1.009330   | 3.073922    |
| 10            | 1             | 0           | 2.431337    | -1.034987   | 3.232082    |
| 11            | 6             | 0           | 4.125550    | 0.539995    | 1.876213    |
| 12            | 6             | 0           | 5.346776    | 0.535043    | 1.969578    |
| 13            | 6             | 0           | 6.699135    | 0.830713    | 2.371082    |
| 14            | 6             | 0           | 6.907683    | 1.893806    | 3.256083    |
| 15            | 6             | 0           | 7.808890    | 0.086710    | 1.914205    |
| 16            | 6             | 0           | 8.186287    | 2.218367    | 3.684502    |
| 17            | 6             | 0           | 9.279774    | 1.482166    | 3.236529    |
| 18            | 6             | 0           | 9.092859    | 0.425180    | 2.359212    |
| 19            | 6             | 0           | 7.670674    | -1.010760   | 1.006563    |
| 20            | 6             | 0           | 7.654671    | -1.956120   | 0.239860    |
| 21            | 6             | 0           | 7.754553    | -3.088735   | -0.629032   |
| 22            | 6             | 0           | 8.990122    | -3.738870   | -0.737087   |
| 23            | 6             | 0           | 9.136008    | -4.846168   | -1.560511   |
| 24            | 6             | 0           | 8.049566    | -5.318920   | -2.290589   |
| 25            | 6             | 0           | 6.819839    | -4.684238   | -2.197600   |
| 26            | 6             | 0           | 6.653512    | -3.567028   | -1.372429   |
| 27            | 6             | 0           | 5.356254    | -2.940813   | -1.328502   |
| 28            | 6             | 0           | 4.191877    | -2.638141   | -1.557023   |
| 29            | 6             | 0           | 2.838587    | -2.301729   | -1.879871   |
| 30            | 6             | 0           | 1.769605    | -2.975572   | -1.278832   |
| 31            | 6             | 0           | 2.566071    | -1.296290   | -2.822628   |
| 32            | 6             | 0           | 0.457343    | -2.647750   | -1.587575   |
| 33            | 6             | 0           | 0.198525    | -1.628366   | -2.507343   |
| 34            | 6             | 0           | 1.263011    | -0.966788   | -3.132760   |
| 35            | 8             | 0           | -1.443606   | 0.481878    | 1.611273    |
| 36            | 8             | 0           | -1.035619   | -1.208211   | -2.870669   |
| 37            | 1             | 0           | 6.052455    | 2.461912    | 3.603765    |
| 38            | 1             | 0           | 8.328256    | 3.046594    | 4.370097    |
| 39            | 1             | 0           | 10.280840   | 1.732359    | 3.570377    |
| 40            | 1             | 0           | 9.940613    | -0.150734   | 2.006028    |
| 41            | 1             | 0           | 9.832092    | -3.366232   | -0.165076   |
| 42            | 1             | 0           | 10.099216   | -5.337883   | -1.631487   |
| 43            | 1             | 0           | 8.159294    | -6.184274   | -2.934988   |
| 44            | 1             | 0           | 5.971059    | -5.047558   | -2.765565   |
| 45            | 1             | 0           | 1.968604    | -3.763746   | -0.560772   |
| 46            | 1             | 0           | 3.386440    | -0.775413   | -3.304367   |
| 47            | 1             | 0           | -0.348876   | -3.188733   | -1.109002   |
| 48            | 1             | 0           | 1.038363    | -0.192227   | -3.857512   |
| 49            | 6             | 0           | -2.191848   | -1.611175   | -2.138845   |
|   |   |   |    |    |    |
|---|---|---|----|----|----|
| 50 | 6 | 0 | -2.197336 | 1.155178 | 0.603377 |
| 51 | 1 | 0 | -2.254713 | -2.702355 | -2.076031 |
| 52 | 1 | 0 | -3.034974 | -1.249539 | -2.726351 |
| 53 | 1 | 0 | -3.237886 | 1.042237 | 0.906394 |
| 54 | 1 | 0 | -1.956401 | 2.221114 | 0.575606 |
| 55 | 6 | 0 | -2.267321 | -0.983840 | -0.745527 |
| 56 | 6 | 0 | -2.020380 | 0.526423 | -0.779700 |
| 57 | 1 | 0 | -1.507967 | -1.424375 | -0.091016 |
| 58 | 1 | 0 | -0.998371 | 0.688078 | -1.136704 |
| 59 | 8 | 0 | -2.946673 | 1.159814 | -1.643463 |
| 60 | 6 | 0 | -1.599236 | 3.116903 | -2.309652 |
| 61 | 6 | 0 | -2.233731 | 4.199597 | -1.667454 |
| 62 | 6 | 0 | -0.236316 | 3.193421 | -2.587978 |
| 63 | 6 | 0 | 0.515514 | 4.312886 | -2.254439 |
| 64 | 6 | 0 | -0.083909 | 5.406419 | -1.628813 |
| 65 | 6 | 0 | -1.473333 | 5.353146 | -1.332134 |
| 66 | 6 | 0 | -3.637648 | 4.188846 | -1.340441 |
| 67 | 6 | 0 | -2.101921 | 6.470226 | -0.700879 |
| 68 | 6 | 0 | -3.488636 | 6.431984 | -0.403581 |
| 69 | 6 | 0 | -4.230257 | 5.249548 | -0.744139 |
| 70 | 6 | 0 | 0.660467 | 6.588231 | -1.279768 |
| 71 | 6 | 0 | 0.062207 | 7.642915 | -0.682351 |
| 72 | 6 | 0 | -1.343142 | 7.624994 | -0.371177 |
| 73 | 6 | 0 | -1.979969 | 8.707113 | 0.241720 |
| 74 | 6 | 0 | -3.339485 | 8.661875 | 0.528786 |
| 75 | 6 | 0 | -4.087967 | 7.536494 | 0.210754 |
| 76 | 1 | 0 | 0.246610 | 2.357462 | -3.08639 |
| 77 | 1 | 0 | 1.575726 | 4.346656 | -2.487569 |
| 78 | 1 | 0 | -4.216111 | 3.299789 | -1.559624 |
| 79 | 1 | 0 | -5.289659 | 5.221260 | -0.506080 |
| 80 | 1 | 0 | 1.720948 | 6.613325 | -1.512896 |
| 81 | 1 | 0 | 0.634152 | 8.530035 | -0.426293 |
| 82 | 1 | 0 | -1.399205 | 9.589973 | 0.492516 |
| 83 | 1 | 0 | -3.818444 | 9.511718 | 1.004449 |
| 84 | 1 | 0 | -5.149741 | 7.504624 | 0.436992 |
| 85 | 6 | 0 | -2.371632 | 1.887719 | -2.728248 |
| 86 | 1 | 0 | -1.720625 | 1.226230 | -3.310238 |
| 87 | 1 | 0 | -3.222130 | 2.160535 | -3.358608 |
| 88 | 8 | 0 | -3.561996 | -1.255696 | -0.240793 |
| 89 | 6 | 0 | -4.987948 | -2.131168 | 1.470829 |
| 90 | 6 | 0 | -5.247209 | -1.543034 | 2.705869 |
| 91 | 6 | 0 | -6.034469 | -2.763006 | 0.772188 |
| 92 | 6 | 0 | -7.331746 | -2.804505 | 1.351231 |
| 93 | 6 | 0 | -7.569900 | -2.202334 | 2.616203 |
| 94 | 6 | 0 | -6.512695 | -1.573916 | 3.274953 |
| 95 | 6 | 0 | -5.843551 | -3.381214 | -0.515048 |
| 96 | 6 | 0 | -6.860044 | -3.998628 | -1.160345 |
| 97 | 6 | 0 | -8.179640 | -4.062355 | -0.595081 |
| 98 | 6 | 0 | -8.404433 | -3.455190 | 0.667441 |
| 99 | 6 | 0 | -8.893355 | -2.260611 | 3.179619 |
| 100 | 6 | 0 | -9.06102 | -2.876891 | 2.530013 |
| 101 | 6 | 0 | -9.700020 | -3.499163 | 1.248414 |
| 102 | 6 | 0 | -10.733301 | -4.143173 | 0.562578 |
| 103 | 6 | 0 | -10.504296 | -4.735863 | -0.673973 |
| 104 | 6 | 0 | -9.240905 | -4.696675 | -1.248779 |
|   |   |   |   |   |
|---|---|---|---|---|
| 105 | 6 | 0 | -3.589006 | -2.087306 | 0.919177 |
| 106 | 1 | 0 | -6.687128 | -1.108795 | 4.240609 |
| 107 | 1 | 0 | -4.866324 | -3.323860 | -0.978766 |
| 108 | 1 | 0 | -6.694916 | -4.456482 | -2.131496 |
| 109 | 1 | 0 | -9.059106 | -1.794608 | 4.146586 |
| 110 | 1 | 0 | -10.900202 | -2.914424 | 2.965995 |
| 111 | 1 | 0 | -11.723421 | -4.176271 | 1.007814 |
| 112 | 1 | 0 | -11.318344 | -5.231878 | -1.192742 |
| 113 | 1 | 0 | -9.065870 | -5.16014 | -2.215404 |
| 114 | 1 | 0 | -2.909533 | -1.682349 | 1.676733 |
| 115 | 1 | 0 | -3.238526 | -3.095788 | 0.657760 |
| 116 | 1 | 0 | -4.435888 | -1.052254 | 3.235849 |
| 117 | 47 | 0 | 5.149795 | -1.186108 | 0.300742 |

SCF Done:  E(RCAM-B3LYP) = -3062.46551674

Full mass-weighted force constant matrix:

Low frequencies --- -2.1559  -0.0014  -0.0010  0.0018  2.8988  4.8087
Low frequencies --- 7.0436  8.2203  12.7871
\( p-(P,S,S)-2:Ag \) : conformer e

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 2.403709    | -0.038210   | -2.199252   |
| 2             | 6             | 0           | 3.743564    | 0.282681    | -2.213587   |
| 3             | 6             | 0           | 1.497939    | 0.751589    | -1.479731   |
| 4             | 6             | 0           | 1.941318    | 1.901515    | -0.824400   |
| 5             | 6             | 0           | 3.293798    | 2.217079    | -0.837141   |
| 6             | 6             | 0           | 4.212759    | 1.406486    | -1.511034   |
| 7             | 1             | 0           | 2.031198    | -0.913231   | -2.719457   |
| 8             | 1             | 0           | 4.444718    | -0.343736   | -2.754893   |
| 9             | 1             | 0           | 1.250572    | 2.541573    | -0.290407   |
| 10            | 1             | 0           | 3.642388    | 3.095838    | -0.305502   |
| 11            | 6             | 0           | 5.617194    | 1.684811    | -1.455620   |
| 12            | 6             | 0           | 6.817042    | 1.922092    | -1.405918   |
| 13            | 6             | 0           | 8.145820    | 2.452695    | -1.564180   |
| 14            | 6             | 0           | 8.296986    | 3.667953    | -2.240387   |
| 15            | 6             | 0           | 9.292922    | 1.791825    | -1.068285   |
| 16            | 6             | 0           | 9.553967    | 4.223749    | -2.426570   |
| 17            | 6             | 0           | 10.683848   | 3.571349    | -1.940889   |
| 18            | 6             | 0           | 10.554435   | 2.365879    | -1.268495   |
| 19            | 6             | 0           | 9.218500    | 0.547103    | -0.363349   |
| 20            | 6             | 0           | 9.260246    | -0.507456   | 0.246109    |
| 21            | 6             | 0           | 9.437468    | -1.745842   | 0.943587    |
| 22            | 6             | 0           | 10.743664   | -2.195977   | 1.172363    |
| 23            | 6             | 0           | 10.973155   | -3.392813   | 1.833205    |
| 24            | 6             | 0           | 9.900215    | -4.160624   | 2.277650    |
| 25            | 6             | 0           | 8.600033    | -3.727657   | 2.063986    |
| 26            | 6             | 0           | 8.347990    | -2.522435   | 1.399813    |
| 27            | 6             | 0           | 6.978265    | -2.118033   | 1.218277    |
| 28            | 6             | 0           | 5.760702    | -1.996039   | 1.256737    |
| 29            | 6             | 0           | 4.336575    | -1.848318   | 1.304287    |
| 30            | 6             | 0           | 3.498302    | -2.741254   | 0.629685    |
| 31            | 6             | 0           | 3.764584    | -0.768389   | 2.000168    |
| 32            | 6             | 0           | 2.123184    | -2.547793   | 0.607995    |
| 33            | 6             | 0           | 1.575203    | -1.438187   | 1.254083    |
| 34            | 6             | 0           | 2.401999    | -0.568100   | 1.976217    |
| 35            | 8             | 0           | 0.222040    | 0.307354    | -1.473538   |
| 36            | 8             | 0           | 0.266095    | -1.107839   | 1.236423    |
| 37            | 1             | 0           | 7.414130    | 4.170217    | -2.618994   |
| 38            | 1             | 0           | 9.650738    | 5.166892    | -2.953105   |
| 39            | 1             | 0           | 11.668407   | 4.002490    | -2.085275   |
| 40            | 1             | 0           | 11.430859   | 1.854218    | -0.887480   |
| 41            | 1             | 0           | 11.575281   | -1.595141   | 0.822296    |
| 42            | 1             | 0           | 11.991152   | -3.727331   | 2.000126    |
| 43            | 1             | 0           | 10.075217   | -5.097854   | 2.794465    |
| 44            | 1             | 0           | 7.761235    | -4.319483   | 2.412219    |
| 45            | 1             | 0           | 3.927464    | -3.587398   | 0.104078    |
| 46            | 1             | 0           | 4.405009    | -0.080704   | 2.542183    |
| 47            | 1             | 0           | 1.495966    | -3.250062   | 0.073586    |
| 48            | 1             | 0           | 1.949310    | 0.272626    | 2.489389    |
| 49            | 6             | 0           | -0.641329   | -1.840528   | 0.419847    |
|   |   |   | 1.754199 | 0.962094 | -0.670843 |
|---|---|---|----------|----------|-----------|
| 6 | 1 | 0  | -0.822987 | -2.826908 | 0.858921  |
| 1 | 1 | 0  | -0.232262 | -1.972967 | -0.585109 |
| 1 | 1 | 0  | -0.375319 | 1.118331  | 0.342760  |
| 1 | 1 | 0  | -0.998154 | 1.935010  | -1.109741 |
| 6 | 1 | 0  | -1.955362 | -1.055857 | 0.377930  |
| 1 | 1 | 0  | -2.105283 | -0.386802 | -0.346445 |
| 8 | 1 | 0  | -3.143380 | 0.842406  | -0.657463 |
| 6 | 1 | 0  | -4.958475 | 2.254990  | -1.054657 |
| 6 | 1 | 0  | -4.947079 | 3.280452  | -0.088877 |
| 6 | 1 | 0  | -6.152431 | 1.934309  | -1.695169 |
| 6 | 1 | 0  | -7.336608 | 2.598873  | -1.405920 |
| 6 | 1 | 0  | -7.362299 | 3.617388  | -0.453038 |
| 6 | 1 | 0  | -6.155993 | 3.965801  | 0.212466  |
| 6 | 1 | 0  | -3.749837 | 3.679646  | 0.607990  |
| 6 | 1 | 0  | -6.165611 | 5.016848  | 1.180793  |
| 6 | 1 | 0  | -4.967065 | 5.384702  | 1.844981  |
| 6 | 1 | 0  |  3.760957 | 4.675677  | 1.520753  |
| 6 | 1 | 0  | -8.571634 | 4.327085  | -0.127784 |
| 6 | 1 | 0  | -8.577984 | 5.317020  | 0.792535  |
| 6 | 1 | 0  | -7.373826 | 5.701374  | 1.480941  |
| 6 | 1 | 0  | -7.359301 | 6.726512  | 2.430490  |
| 6 | 1 | 0  | -6.180784 | 7.079102  | 3.077705  |
| 6 | 1 | 0  | -4.995245 | 6.416279  | 2.788975  |
| 6 | 1 | 0  | -6.153913 | 1.145544  | -2.441624 |
| 6 | 1 | 0  | -8.252256 | 2.329033  | -1.924143 |
| 6 | 1 | 0  | -2.832675 | 3.138495  | 0.406103  |
| 6 | 1 | 0  | -2.845520 | 4.957360  | 2.034574  |
| 6 | 1 | 0  | -9.485078 | 4.045712  | -0.643518 |
| 6 | 1 | 0  | -9.496883 | 5.845145  | 1.029799  |
| 6 | 1 | 0  | -8.283837 | 7.248855  | 2.658714  |
| 6 | 1 | 0  | -6.187554 | 7.877710  | 3.812681  |
| 6 | 1 | 0  | -4.076165 | 6.694776  | 3.296429  |
| 6 | 1 | 0  | -3.701880 | 1.530748  | -1.460387 |
| 6 | 1 | 0  | -2.971545 | 2.243423  | -1.869334 |
| 6 | 1 | 0  | -3.933446 | 0.810137  | -2.254349 |
| 6 | 1 | 0  | -3.006593 | -1.945368 | 0.058209  |
| 6 | 1 | 0  | -4.636260 | -3.553586 | 0.766026  |
| 6 | 1 | 0  | -4.403807 | -4.912934 | 0.955487  |
| 6 | 1 | 0  | -5.853525 | -3.130360 | 0.199421  |
| 6 | 1 | 0  | -6.834651 | -4.101614 | -0.139890 |
| 6 | 1 | 0  | -6.575241 | -5.483723 | 0.065059  |
| 6 | 1 | 0  | -5.349274 | -5.867839 | 0.609431  |
| 6 | 1 | 0  | -6.153739 | -1.740895 | -0.40003  |
| 6 | 1 | 0  | -7.350647 | -1.359097 | -0.543583 |
| 6 | 1 | 0  | -8.367642 | -2.317044 | -0.879817 |
| 6 | 1 | 0  | -8.092775 | -3.694352 | -0.680576 |
| 6 | 1 | 0  | -7.586878 | -6.444682 | -0.289353 |
| 6 | 1 | 0  | -8.775405 | -6.055803 | -0.802883 |
| 6 | 1 | 0  | -9.075392 | -4.664129 | -1.015163 |
| 6 | 1 | 0  | -10.301208| -4.240992 | -1.535947 |
| 6 | 1 | 0  | -10.563357| -2.889213 | -1.726540 |
| 6 | 1 | 0  | -9.607493 | -1.935323 | -1.402553 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 105 | 6 | 0 | -3.593288 | -2.561188 | 1.199986 |
| 106 | 1 | 0 | -5.142715 | -6.922046 | 0.768457 |
| 107 | 1 | 0 | -5.390487 | -0.997106 | 0.160938 |
| 108 | 1 | 0 | -7.559334 | -0.306858 | -0.711247 |
| 109 | 1 | 0 | -7.371449 | -7.497284 | -0.130205 |
| 110 | 1 | 0 | -9.531486 | -6.790532 | -1.064124 |
| 111 | 1 | 0 | -11.052200 | -4.983186 | -1.790683 |
| 112 | 1 | 0 | -11.521180 | -2.577844 | -2.131187 |
| 113 | 1 | 0 | -9.815648 | -0.879972 | -1.553580 |
| 114 | 1 | 0 | -2.827624 | -3.078258 | 1.792310 |
| 115 | 1 | 0 | -4.031497 | -1.783489 | 1.840584 |
| 116 | 1 | 0 | -3.460967 | -5.230077 | 1.391939 |
| 117 | 47 | 0 | 6.730366 | -0.094626 | -0.080744 |

SCF Done:  E(RCAM-B3LYP) = -3062.46549106  A.U. after 5 cycles
Full mass-weighted force constant matrix:
Low frequencies --- -1.7408 -0.0099 -0.0004  0.0072  2.3064  4.0251
Low frequencies ---  6.2744  7.1141  9.7712
**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -2.390676   | -0.228994  | -2.145433   |
| 2             | 6             | 0           | -3.751296   | -0.443641  | -2.146190   |
| 3             | 6             | 0           | -1.525208   | -1.196009  | -1.617949   |
| 4             | 6             | 0           | -2.034978   | -2.480126  | -1.149154   |
| 5             | 6             | 0           | -3.408246   | -2.616812  | -1.146636   |
| 6             | 6             | 0           | -4.283316   | -1.635449  | -1.623179   |
| 7             | 1             | 0           | -1.968265   | 0.694256   | -0.770194   |
| 8             | 1             | 0           | -4.420119   | 0.317290   | -2.534644   |
| 9             | 1             | 0           | -1.378248   | -3.180927  | -0.770194   |
| 10            | 1             | 0           | -3.806495   | -3.547142  | -0.756360   |
| 11            | 6             | 0           | -5.702794   | -1.810658  | -1.542234   |
| 12            | 6             | 0           | -6.916106   | -1.956593  | -1.470088   |
| 13            | 6             | 0           | -8.287862   | -2.358375  | -1.641139   |
| 14            | 6             | 0           | -8.557519   | -3.461128  | -2.458688   |
| 15            | 6             | 0           | -9.362535   | -1.680753  | -1.021130   |
| 16            | 6             | 0           | -9.860630   | -3.888972  | -2.664475   |
| 17            | 6             | 0           | -10.919172  | -3.218351  | -2.057835   |
| 18            | 6             | 0           | -10.672248  | -2.123535  | -1.243969   |
| 19            | 6             | 0           | -9.165309   | -0.550619  | -0.163293   |
| 20            | 6             | 0           | -9.100401   | 0.410800   | 0.583400    |
| 21            | 6             | 0           | -9.156835   | 1.547653   | 1.453517    |
| 22            | 6             | 0           | -10.414987  | 2.063805   | 1.787442    |
| 23            | 6             | 0           | -10.528187  | 3.167057   | 2.619291    |
| 24            | 6             | 0           | -9.384977   | 3.773012   | 3.133138    |
| 25            | 6             | 0           | -8.130879   | 3.272552   | 2.816326    |
| 26            | 6             | 0           | -7.995858   | 2.160285   | 1.978643    |
| 27            | 6             | 0           | -6.669523   | 1.680879   | 1.690001    |
| 28            | 6             | 0           | -5.467477   | 1.452690   | 1.649880    |
| 29            | 6             | 0           | -4.060431   | 1.185955   | 1.603099    |
| 30            | 6             | 0           | -3.176206   | 2.109509   | 1.036965    |
| 31            | 6             | 0           | -3.554423   | -0.031733  | 2.093040    |
| 32            | 6             | 0           | -1.822796   | 1.820221   | 0.921150    |
| 33            | 6             | 0           | -1.344368   | 0.585837   | 1.362972    |
| 34            | 6             | 0           | -2.213688   | -0.325281  | 1.976171    |
| 35            | 8             | 0           | -0.219817   | -0.851464  | -1.598624   |
| 36            | 8             | 0           | -0.065714   | 0.169374   | 1.239409    |
| 37            | 1             | 0           | -7.729909   | -3.977439  | -2.931534   |
| 38            | 1             | 0           | -10.049377  | -4.746222  | -3.301366   |
| 39            | 1             | 0           | -11.939463  | -3.549295  | -2.217714   |
| 40            | 1             | 0           | -11.492567  | -1.598744  | -0.767727   |
| 41            | 1             | 0           | -11.301733  | 1.589167   | 1.383053    |
| 42            | 1             | 0           | -11.510440  | 3.555055   | 2.865714    |
| 43            | 1             | 0           | -9.469167   | 4.636574   | 3.783736    |
| 44            | 1             | 0           | -7.237755   | 3.738664   | 3.216477    |
| 45            | 1             | 0           | -3.553497   | 3.058153   | 0.670645    |
| 46            | 1             | 0           | -4.228646   | -0.748520  | 2.549842    |
| 47            | 1             | 0           | -1.158888   | 2.548801   | 0.473293    |
| 48            | 1             | 0           | -1.812719   | -1.268097  | 2.330225    |
| 49            | 6             | 0           | 0.868441    | 0.948591   | 0.500587    |
| 50 | 6 | 0 | 0.733419 | -1.701539 | -0.969156 |
| 51 | 1 | 0 | 1.125107 | 1.850192  | 1.067124  |
| 52 | 1 | 0 | 0.445164 | 1.244371  | -0.462835 |
| 53 | 1 | 0 | 0.374906 | -2.018607 | 0.014018  |
| 54 | 1 | 0 | 0.916759 | -2.585819 | -1.587217 |
| 55 | 6 | 0 | 2.111557 | 0.075264  | 0.311182  |
| 56 | 6 | 0 | 2.039006 | -0.914258 | -0.858951 |
| 57 | 1 | 0 | 2.260393 | -0.504887 | 1.232522  |
| 58 | 1 | 0 | 2.163722 | -0.346185 | -1.798678 |
| 59 | 8 | 0 | 3.073829 | -1.869473 | -0.713546 |
| 60 | 6 | 0 | 5.176261 | -2.804131 | -1.373676 |
| 61 | 6 | 0 | 5.848693 | -2.958526 | -0.149008 |
| 62 | 6 | 0 | 5.434880 | -3.675321 | -2.428160 |
| 63 | 6 | 0 | 6.348062 | -4.713993 | -2.307653 |
| 64 | 6 | 0 | 7.036299 | -4.917791 | -1.112262 |
| 65 | 6 | 0 | 6.785417 | -4.054791 | -0.017808 |
| 66 | 6 | 0 | 5.627105 | -2.128047 | 0.985754  |
| 67 | 6 | 0 | 7.484215 | -4.239184 | 1.213707  |
| 68 | 6 | 0 | 7.244446 | -3.373920 | 2.312611  |
| 69 | 6 | 0 | 6.288839 | -2.312441 | 2.151780  |
| 70 | 6 | 0 | 7.992199 | -5.982129 | -0.950392 |
| 71 | 6 | 0 | 8.651407 | -6.162976 | 0.215935  |
| 72 | 6 | 0 | 8.422907 | -5.297459 | 1.343405  |
| 73 | 6 | 0 | 9.095592 | -5.467238 | 2.556553  |
| 74 | 6 | 0 | 8.854239 | -4.615445 | 3.628163  |
| 75 | 6 | 0 | 7.937913 | -3.578696 | 3.509696  |
| 76 | 1 | 0 | 4.910980 | -3.533995 | -3.369098 |
| 77 | 1 | 0 | 6.532084 | -5.376687 | -3.148105 |
| 78 | 1 | 0 | 4.897082 | -1.334278 | 0.893004  |
| 79 | 1 | 0 | 6.101272 | -1.657181 | 2.998194  |
| 80 | 1 | 0 | 8.172759 | -6.640555 | -1.795085 |
| 81 | 1 | 0 | 9.370653 | -6.969603 | 0.324520  |
| 82 | 1 | 0 | 9.813507 | -6.276388 | 2.654395  |
| 83 | 1 | 0 | 9.385722 | -4.761587 | 4.563169  |
| 84 | 1 | 0 | 7.752139 | -2.915250 | 4.349420  |
| 85 | 6 | 0 | 4.199422 | -1.675038 | -1.568956 |
| 86 | 1 | 0 | 3.686865 | -1.655901 | -2.615218 |
| 87 | 1 | 0 | 4.661265 | -0.706796 | -1.346338 |
| 88 | 8 | 0 | 3.245230 | 0.885631  | 0.051607  |
| 89 | 6 | 0 | 5.095663 | 2.208503  | 0.789745  |
| 90 | 6 | 0 | 6.350723 | 1.729119  | 1.154800  |
| 91 | 6 | 0 | 4.999196 | 3.407699  | 0.057305  |
| 92 | 6 | 0 | 6.184967 | 4.117366  | -0.274723 |
| 93 | 6 | 0 | 7.454154 | 3.611268  | 0.115555  |
| 94 | 6 | 0 | 7.513344 | 2.412099  | 0.825872  |
| 95 | 6 | 0 | 3.737219 | 3.955541  | -0.370417 |
| 96 | 6 | 0 | 3.666810 | 5.121519  | -1.053341 |
| 97 | 6 | 0 | 4.848434 | 5.865898  | -1.391537 |
| 98 | 6 | 0 | 6.109135 | 5.347581  | -0.997795 |
| 99 | 6 | 0 | 8.638915 | 4.351249  | -0.232567 |
| 100 | 6 | 0 | 8.563707 | 5.515024  | -0.916128 |
| 101 | 6 | 0 | 7.294814 | 6.058914  | -1.323796 |
| 102 | 6 | 0 | 7.196270 | 7.262304  | -2.027320 |
| 103 | 6 | 0 | 5.956960 | 7.763380  | -2.408464 |
| 104 | 6 | 0 | 4.793388 | 7.073243  | -2.095374 |
|   |   |   |    3.866154 |  1.445722 |  1.205128 |
|---|---|---|-------------|-----------|-----------|
|106| 1 | 0 |  8.479347   |  2.015661 |  1.123840 |
|107| 1 | 0 |  2.831342   |  3.401196 | -0.157691 |
|108| 1 | 0 |  2.704260   |  5.515626 | -1.366916 |
|109| 1 | 0 |  9.601200   |  3.949259 |  0.070788 |
|110| 1 | 0 |  9.464810   |  6.064825 | -1.171861 |
|111| 1 | 0 |  8.103391   |  7.805884 | -2.274887 |
|112| 1 | 0 |  5.898843   |  8.699530 | -2.954593 |
|113| 1 | 0 |  3.826942   |  7.467180 | -2.396224 |
|114| 1 | 0 |  3.164666   |  2.105166 |  1.733070 |
|115| 1 | 0 |  4.142783   |  0.643080 |  1.900233 |
|116| 1 | 0 |  6.421312   |  0.797313 |  1.708027 |
|117| 47| 0 | -6.641478   | -0.134370 |  0.096169 |

SCF Done:  E(RCAM-B3LYP) = -3062.46444371
Full mass-weighted force constant matrix:
Low frequencies ---  -1.1166  -0.0079  -0.0009  0.0078  3.0234
5.0156
Low frequencies ---  7.3356   8.2107  12.0762
### $p$-(P,S)-2:Ag: conformer f

#### Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -0.019444   | 0.238698   | 1.711220    |
| 2             | 6             | 0           | -1.219612   | -0.366885  | 2.054617    |
| 3             | 6             | 0           | -0.030218   | 1.491356   | 1.092018    |
| 4             | 6             | 0           | -1.248949   | 2.137082   | 0.843467    |
| 5             | 6             | 0           | -2.438482   | 1.531760   | 1.188614    |
| 6             | 6             | 0           | -2.441351   | 0.262770   | 1.793303    |
| 7             | 1             | 0           | 0.910679    | -0.270987  | 1.928088    |
| 8             | 1             | 0           | -1.209541   | -1.341571  | 2.530429    |
| 9             | 1             | 0           | -1.229233   | 3.111463   | 0.367720    |
| 10            | 1             | 0           | -3.379951   | 2.032489   | 0.989122    |
| 11            | 6             | 0           | -3.679167   | -0.364612  | 2.144371    |
| 12            | 6             | 0           | -4.747320   | -0.865451  | 2.474555    |
| 13            | 6             | 0           | -5.904216   | -1.288449  | 3.222904    |
| 14            | 6             | 0           | -5.908227   | -1.082368  | 4.606502    |
| 15            | 6             | 0           | -7.028178   | -1.887787  | 2.612191    |
| 16            | 6             | 0           | -6.999626   | -1.458177  | 5.375563    |
| 17            | 6             | 0           | -8.108983   | -2.044671  | 4.772600    |
| 18            | 6             | 0           | -8.123423   | -2.257166  | 3.402730    |
| 19            | 6             | 0           | -7.091262   | -2.137323  | 1.204009    |
| 20            | 6             | 0           | -7.236801   | -2.395733  | 0.023016    |
| 21            | 6             | 0           | -7.518983   | -2.721331  | -1.342026   |
| 22            | 6             | 0           | -8.813754   | -3.138835  | -1.673816   |
| 23            | 6             | 0           | -9.138035   | -3.460529  | -2.982829   |
| 24            | 6             | 0           | -8.173330   | -3.371107  | -3.982628   |
| 25            | 6             | 0           | -6.884986   | -2.963102  | -3.670407   |
| 26            | 6             | 0           | -6.538830   | -2.634739  | -2.355494   |
| 27            | 6             | 0           | -5.181273   | -2.232033  | -2.088729   |
| 28            | 6             | 0           | -3.984827   | -1.989585  | -2.187321   |
| 29            | 6             | 0           | -2.580520   | -1.750883  | -2.328713   |
| 30            | 6             | 0           | -1.654048   | -2.728171  | -1.926596   |
| 31            | 6             | 0           | -2.107280   | -0.550348  | -2.868662   |
| 32            | 6             | 0           | -0.300483   | -2.495647  | -2.046735   |
| 33            | 6             | 0           | 0.166051    | -1.281661  | -2.568030   |
| 34            | 6             | 0           | -0.745782   | -0.311938  | -2.992654   |
| 35            | 8             | 0           | 1.068307    | 2.173475   | 0.700149    |
| 36            | 8             | 0           | 1.512203    | -1.160603  | -2.616164   |
| 37            | 1             | 0           | -5.043236   | -0.622461  | 5.070590    |
| 38            | 1             | 0           | -6.983841   | -1.291058  | 6.446972    |
| 39            | 1             | 0           | -8.964570   | -2.338695  | 5.370631    |
| 40            | 1             | 0           | -8.983690   | -2.715112  | 2.928076    |
| 41            | 1             | 0           | -9.561386   | -3.205039  | -0.891748   |
| 42            | 1             | 0           | -10.145997  | -3.780612  | -3.223058   |
| 43            | 1             | 0           | -8.423145   | -3.620956  | -5.007980   |
| 44            | 1             | 0           | -6.128928   | -2.895063  | -4.444270   |
| 45            | 1             | 0           | -2.008436   | -3.667607  | -1.516284   |
| 46            | 1             | 0           | -2.813214   | 0.207257   | -3.191277   |
| 47            | 1             | 0           | 0.425664    | -3.238516  | -1.736607   |
| 48            | 1             | 0           | -0.413526   | 0.628228   | -3.413828   |
| 49            | 6             | 0           | 2.132916    | 0.076689   | -2.958094   |
|   |   |   |   |     |     |     |
|---|---|---|---|-----|-----|-----|
| 50 | 6 | 0 | 2.345893 | 1.547244 | 0.644041 |
| 51 | 1 | 0 | 1.734215 | 0.460435 | -3.902576 |
| 52 | 1 | 0 | 3.184360 | -0.169601 | -3.100248 |
| 53 | 1 | 0 | 3.046865 | 2.360167 | 0.461566 |
| 54 | 1 | 0 | 2.598535 | 1.078398 | 1.600683 |
| 55 | 6 | 0 | 2.036191 | 1.125031 | -1.841953 |
| 56 | 6 | 0 | 2.451465 | 0.533608 | -0.497677 |
| 57 | 1 | 0 | 1.009924 | 1.493212 | -1.736342 |
| 58 | 8 | 0 | 3.976653 | 0.106762 | -0.577876 |
| 59 | 6 | 0 | 5.534220 | -1.466084 | -0.802695 |
| 60 | 6 | 0 | 6.046970 | -2.660347 | -0.428136 |
| 61 | 6 | 0 | 6.389809 | -0.581014 | -0.759935 |
| 62 | 6 | 0 | 7.746057 | -0.852493 | -0.883117 |
| 63 | 6 | 0 | 8.292398 | -2.023519 | -0.358561 |
| 64 | 6 | 0 | 7.434556 | -2.940585 | 0.305706 |
| 65 | 6 | 0 | 5.217478 | -3.621992 | 1.109431 |
| 66 | 6 | 0 | 7.976531 | -4.145129 | 0.850647 |
| 67 | 6 | 0 | 7.131228 | -5.070109 | 1.516897 |
| 68 | 6 | 0 | 5.731799 | -4.763046 | 1.624593 |
| 69 | 6 | 0 | 9.694351 | -2.331477 | -0.467330 |
| 70 | 6 | 0 | 10.205162 | -3.471414 | 0.049359 |
| 71 | 6 | 0 | 9.364810 | -4.422572 | 0.728878 |
| 72 | 6 | 0 | 9.872865 | -5.606258 | 1.270610 |
| 73 | 6 | 0 | 9.037580 | -6.506690 | 1.921862 |
| 74 | 6 | 0 | 7.679811 | -6.243457 | 2.044968 |
| 75 | 6 | 0 | 5.979231 | -3.333332 | -1.169468 |
| 76 | 1 | 0 | 8.394240 | -0.145381 | -1.392804 |
| 77 | 1 | 0 | 4.155360 | -3.427584 | 1.211101 |
| 78 | 1 | 0 | 5.087020 | -5.473402 | 2.133974 |
| 79 | 1 | 0 | 10.336780 | -1.619917 | -0.977955 |
| 80 | 1 | 0 | 11.264901 | -3.692405 | -0.038649 |
| 81 | 1 | 0 | 10.934258 | -5.817287 | 1.177455 |
| 82 | 1 | 0 | 9.449840 | -7.421055 | 2.336659 |
| 83 | 1 | 0 | 7.030358 | -6.949308 | 2.554637 |
| 84 | 6 | 0 | 4.062740 | -1.149930 | 0.010787 |
| 85 | 1 | 0 | 3.768928 | -1.143702 | 1.070837 |
| 86 | 1 | 0 | 3.460233 | -1.923756 | -0.487343 |
| 87 | 8 | 0 | 2.909225 | -2.191653 | -2.161896 |
| 88 | 6 | 0 | 1.376864 | 4.117895 | -2.250930 |
| 89 | 6 | 0 | 0.049235 | 4.162971 | -2.66654 |
| 90 | 1 | 0 | 1.790358 | 4.925224 | -1.172573 |
| 91 | 6 | 0 | 0.5843513 | 5.767859 | -0.530789 |
| 92 | 6 | 0 | -0.508242 | 5.792118 | -0.971416 |
| 93 | 6 | 0 | -0.883788 | 4.981553 | -2.043358 |
| 94 | 6 | 0 | 3.149601 | 4.939706 | -0.693946 |
| 95 | 6 | 0 | 3.526590 | 5.731092 | 0.337731 |
| 96 | 6 | 0 | 2.589756 | 6.590848 | 1.006038 |
| 97 | 6 | 0 | 1.243231 | 6.600582 | 0.559411 |
| 98 | 6 | 0 | -1.446233 | 6.656160 | -0.302675 |
| 99 | 6 | 0 | -1.064477 | 7.440317 | 0.729984 |
| 100 | 6 | 0 | 0.295938 | 7.442934 | 1.200626 |
| 101 | 6 | 0 | 0.709672 | 8.248361 | 2.264675 |
| 102 | 6 | 0 | 2.031043 | 8.232018 | 2.696581 |
| 103 | 6 | 0 | 2.963361 | 7.412437 | 2.074763 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|105| 6 | 0 | 2.351638| 3.221618| -2.976689|
|106| 1 | 0 | -1.912414| 4.999507| -2.391513|
|107| 1 | 0 | 3.875987 | 4.288327| -1.164798|
|108| 1 | 0 | 4.556806 | 5.727460| 0.681908 |
|109| 1 | 0 | -2.474539| 6.664179| -0.652197|
|110| 1 | 0 | -1.781112| 8.088643| 1.225796 |
|111| 1 | 0 | -0.015435| 8.892303| 2.753769 |
|112| 1 | 0 | 2.335310 | 8.864484| 3.524438 |
|113| 1 | 0 | 3.995011 | 7.402861| 2.414249 |
|114| 1 | 0 | 1.863617 | 2.790492| -3.858768|
|115| 1 | 0 | 3.214836 | 3.790438| -3.318114|
|116| 1 | 0 | -0.260363| 3.548809| -3.508104|
|117| 47| 0 | -4.793539| -1.480808| 0.160444|

SCF Done:  E(RCAM-B3LYP) = -3062.46419642
Full mass-weighted force constant matrix:
Low frequencies ---  -10.9423  -5.8656  -0.0018  -0.0008  -0.0005 2.2517
Low frequencies ---  6.4928  7.5030  10.4515

S74
Principal conformers of compound \(p\,(P,S,S)-3\) in absence and presence of Ag.

\(p\,(P,S,S)-3\): conformer a

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 1.753482   | -1.704482  | -1.786891  |
| 2             | 6             | 0           | 3.042697   | -2.177034  | -1.577686  |
| 3             | 6             | 0           | 1.557324   | -0.347544  | -2.042346  |
| 4             | 6             | 0           | 2.653298   | 0.515030   | -2.120935  |
| 5             | 6             | 0           | 3.931639   | 0.037009   | -1.906213  |
| 6             | 6             | 0           | 4.146400   | -1.318919  | -1.615722  |
| 7             | 6             | 0           | 0.919018   | -2.391848  | -1.711501  |
| 8             | 6             | 0           | 3.193922   | -3.228527  | -1.358094  |
| 9             | 6             | 0           | 2.475482   | 1.564919   | -2.326294  |
| 10            | 6             | 0           | 4.776462   | 0.716277   | -1.936481  |
| 11            | 6             | 0           | 5.454512   | -1.808135  | -1.317350  |
| 12            | 6             | 0           | 6.551458   | -2.228252  | -1.028827  |
| 13            | 6             | 0           | 7.818476   | -2.801924  | -0.709057  |
| 14            | 6             | 0           | 7.995611   | -4.85347   | -0.845151  |
| 15            | 6             | 0           | 8.900668   | -2.013437  | -0.258608  |
| 16            | 6             | 0           | 9.211068   | -4.782231  | -0.549873  |
| 17            | 6             | 0           | 10.280003  | -4.038057  | -0.112382  |
| 18            | 6             | 0           | 10.123377  | -2.634120  | 0.030088   |
| 19            | 6             | 0           | 8.791325   | -0.598784  | -0.088635  |
| 20            | 6             | 0           | 8.791413   | 0.597663   | 0.088773   |
| 21            | 6             | 0           | 8.901029   | 2.012307   | 0.258640   |
| 22            | 6             | 0           | 10.123844  | 2.632739   | -0.030146  |
| 23            | 6             | 0           | 10.280738  | 4.002403   | 0.112238   |
| 24            | 6             | 0           | 9.211970   | 4.781058   | 0.549727   |
| 25            | 6             | 0           | 7.996411   | 4.184423   | 0.845095   |
| 26            | 6             | 0           | 7.819007   | 2.801028   | 0.709093   |
| 27            | 6             | 0           | 6.551891   | 2.227623   | 1.028965   |
| 28            | 6             | 0           | 5.454911   | 1.807596   | 1.317494   |
| 29            | 6             | 0           | 4.146756   | 1.318444   | 1.615776   |
| 30            | 6             | 0           | 3.043120   | 2.176649   | 1.577877   |
| 31            | 6             | 0           | 3.931894   | -0.037512  | 1.906076   |
| 32            | 6             | 0           | 1.753871   | 1.704166   | 1.787046   |
| 33            | 6             | 0           | 1.557611   | 0.347207   | 2.042301   |
| 34            | 6             | 0           | 2.653518   | -0.515466  | 2.120745   |
| 35            | 8             | 0           | 0.337742   | 0.240815   | -2.225079  |
| 36            | 8             | 0           | 0.337988   | -0.241074  | 2.225019   |
| 37            | 1             | 0           | 7.160365   | -4.784969  | -1.190141  |
| 38            | 1             | 0           | 9.325825   | -5.855260  | -0.662827  |
| 39            | 1             | 0           | 11.234708  | -4.464478  | 0.118863   |
| 40            | 1             | 0           | 10.949665  | -2.021089  | 0.373181   |
| 41            | 1             | 0           | 10.950003  | 2.019530   | -0.373232  |
| 42            | 1             | 0           | 11.235522  | 4.462882   | -0.119069  |
| 43            | 1             | 0           | 9.326932   | 5.854072   | 0.662606   |
| 44            | 1             | 0           | 7.161295   | 4.784227   | 1.190084   |
| 45            | 1             | 0           | 3.194423   | 3.228165   | 1.358451   |
| 46            | 1             | 0           | 4.776671   | -0.716841  | 1.936249   |
| 47            | 1             | 0           | 0.919460   | 2.391613   | 1.711800   |
|   |   |   |     |     |     |
|---|---|---|-----|-----|-----|
| 48 | 1 | 0 | 2.475622 | -1.565369 | 2.325967 |
| 49 | 6 | 0 | -0.842818 | 0.470217 | 1.891554 |
| 50 | 6 | 0 | -0.843105 | -0.472169 | -1.891544 |
| 51 | 1 | 0 | -0.880325 | 1.442475 | 2.395391 |
| 52 | 1 | 0 | -1.666005 | -0.142430 | 2.259264 |
| 53 | 1 | 0 | -1.666267 | -0.472169 | -2.259196 |
| 54 | 1 | 0 | -0.880734 | 1.442475 | 2.393591 |
| 55 | 6 | 0 | -0.970304 | 0.657466 | 0.378406 |
| 56 | 6 | 0 | -0.970474 | -0.657605 | -0.378389 |
| 57 | 1 | 0 | -0.139648 | 1.257243 | 0.005047 |
| 58 | 1 | 0 | -0.139897 | -1.257550 | -0.005122 |
| 59 | 8 | 0 | -2.197028 | -1.338355 | -0.093368 |
| 60 | 6 | 0 | -3.485752 | -3.279705 | 0.225062 |
| 61 | 6 | 0 | -3.774497 | -4.562177 | 0.519820 |
| 62 | 6 | 0 | -4.447317 | -3.431550 | 0.787628 |
| 63 | 6 | 0 | -5.679677 | -2.903809 | 1.190114 |
| 64 | 6 | 0 | -6.006304 | -4.253438 | 1.386433 |
| 65 | 6 | 0 | -5.052866 | -5.136438 | 0.464569 |
| 66 | 6 | 0 | -2.858354 | -5.605451 | -0.529890 |
| 67 | 6 | 0 | -5.393930 | -6.515962 | 0.306626 |
| 68 | 6 | 0 | -4.446821 | -7.419294 | -0.266017 |
| 69 | 6 | 0 | -3.190483 | -6.908990 | -0.677980 |
| 70 | 6 | 0 | -7.285331 | -4.763063 | 1.450324 |
| 71 | 6 | 0 | -7.600191 | -6.068785 | 1.299186 |
| 72 | 6 | 0 | -6.665718 | -6.993990 | 0.720691 |
| 73 | 6 | 0 | -6.976000 | -8.346549 | 0.556196 |
| 74 | 6 | 0 | -6.057322 | -9.223939 | 0.006056 |
| 75 | 6 | 0 | -4.812360 | -8.765441 | -0.414079 |
| 76 | 1 | 0 | -4.212162 | -1.382580 | 0.910799 |
| 77 | 1 | 0 | -6.404712 | -2.225511 | 1.628862 |
| 78 | 1 | 0 | -1.888406 | -5.253623 | -0.845686 |
| 79 | 1 | 0 | -2.479419 | -7.600671 | -1.120771 |
| 80 | 1 | 0 | -7.995690 | -4.068115 | 1.887653 |
| 81 | 1 | 0 | -8.569803 | -6.443792 | 1.613407 |
| 82 | 1 | 0 | -7.949663 | -8.706909 | 0.875006 |
| 83 | 1 | 0 | -6.314317 | -10.271337 | -0.126442 |
| 84 | 1 | 0 | -4.094131 | -9.451157 | -0.853932 |
| 85 | 6 | 0 | -2.180369 | -2.689162 | -0.165753 |
| 86 | 8 | 0 | -1.182736 | -3.289633 | -0.513804 |
| 87 | 8 | 0 | -2.196750 | 1.338457 | 0.093500 |
| 88 | 6 | 0 | -2.179812 | 2.689259 | 0.165874 |
| 89 | 8 | 0 | -1.181969 | 3.289536 | 0.513660 |
| 90 | 6 | 0 | -3.485091 | 3.280066 | -0.224894 |
| 91 | 6 | 0 | -3.773487 | 4.656671 | -0.051973 |
| 92 | 6 | 0 | -4.446914 | 2.432067 | -0.787253 |
| 93 | 6 | 0 | -5.051785 | 5.137142 | -0.464493 |
| 94 | 6 | 0 | -2.857057 | 5.605767 | 0.529674 |
| 95 | 6 | 0 | -5.679204 | 2.904566 | -1.189675 |
| 96 | 1 | 0 | -4.212024 | 1.383024 | -0.910307 |
| 97 | 6 | 0 | -5.392503 | 6.516769 | -0.306705 |
| 98 | 6 | 0 | -6.005493 | 4.254292 | -1.038349 |
| 99 | 6 | 0 | -3.188858 | 6.909406 | 0.677526 |
| 100 | 1 | 0 | -1.887161 | 5.253749 | 0.845419 |
| 101 | 1 | 0 | -6.404446 | 2.226383 | -1.628259 |
| 102 | 6 | 0 | -4.463116 | 7.419958 | 0.265714 |
|   |   |   |            |            |            |
|---|---|---|------------|------------|------------|
| 103| 6 | 0 | -6.664218  | 6.995045   | -0.720704  |
| 104| 6 | 0 | -7.284440  | 4.764167   | -1.449966  |
| 105| 1 | 0 | -2.477584  | 7.600978   | 1.120238   |
| 106| 6 | 0 | -4.810315  | 8.766210   | 0.413623   |
| 107| 6 | 0 | -6.974157  | 8.347703   | -0.556368  |
| 108| 6 | 0 | -7.598974  | 6.069985   | -1.298974  |
| 109| 1 | 0 | -7.995011  | 4.069329   | -1.887128  |
| 110| 6 | 0 | -6.055209  | 9.224951   | 0.005665   |
| 111| 1 | 0 | -4.091874  | 9.451814   | 0.853304   |
| 112| 1 | 0 | -7.947765  | 8.708254   | -0.875129  |
| 113| 1 | 0 | -8.568529  | 6.445179   | -1.613145  |
| 114| 1 | 0 | -6.311939  | 10.272428  | 0.125929   |

SCF Done: \( E({\text{RCAM-B3LYP}}) = -3065.01143051 \)

Full mass-weighted force constant matrix:

Low frequencies --- -3.4064 -0.0030 -0.0019 -0.0002 2.7133 3.3141

Low frequencies --- 5.4080 8.4125 9.0840
\[ p-(P,S)-3:Ag : \text{conformer } b \]

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -3.273943  | -3.007921  | -1.497917   |
| 2             | 6             | 0           | -4.650853  | -3.070770  | -1.324164   |
| 3             | 6             | 0           | -2.511588  | -2.220609  | -0.637121   |
| 4             | 6             | 0           | -3.120561  | -1.559427  | 0.432107    |
| 5             | 6             | 0           | -4.489317  | -1.622986  | 0.595346    |
| 6             | 6             | 0           | -5.281659  | -2.362113  | -0.297304   |
| 7             | 1             | 0           | -2.811992  | -3.558031  | -2.308803   |
| 8             | 1             | 0           | -5.249083  | -3.662552  | -2.008841   |
| 9             | 1             | 0           | -2.503588  | -0.964096  | 1.095776    |
| 10            | 1             | 0           | -4.965230  | -1.073284  | 1.399944    |
| 11            | 6             | 0           | -6.705680  | -2.344709  | -0.190775   |
| 12            | 6             | 0           | -7.912183  | -2.286823  | -0.131912   |
| 13            | 6             | 0           | -9.338656  | -2.283222  | -0.100025   |
| 14            | 6             | 0           | -10.037344 | -3.400332  | -0.574785   |
| 15            | 6             | 0           | -10.06690  | -1.177225  | 0.393850    |
| 16            | 6             | 0           | -11.422706 | -3.436117  | -0.561087   |
| 17            | 6             | 0           | -12.140900 | -2.349341  | -0.068127   |
| 18            | 6             | 0           | -11.467262 | -1.234077  | 0.403939    |
| 19            | 6             | 0           | -9.431932  | 0.003082   | 0.891639    |
| 20            | 6             | 0           | -9.012004  | 1.047558   | 1.335249    |
| 21            | 6             | 0           | -8.661464  | 2.287834   | 1.954030    |
| 22            | 6             | 0           | -9.566006  | 2.844989   | 2.869344    |
| 23            | 6             | 0           | -9.290788  | 4.041799   | 3.510641    |
| 24            | 6             | 0           | -8.097825  | 4.710314   | 3.246344    |
| 25            | 6             | 0           | -7.193651  | 4.177885   | 2.341499    |
| 26            | 6             | 0           | -7.454788  | 2.968873   | 1.681271    |
| 27            | 6             | 0           | -6.485408  | 2.470709   | 0.759088    |
| 28            | 6             | 0           | -5.602690  | 2.133945   | 0.003462    |
| 29            | 6             | 0           | -4.535346  | 1.717675   | -0.850016   |
| 30            | 6             | 0           | -3.224344  | 2.133944   | -0.597550   |
| 31            | 6             | 0           | -4.767411  | 0.850883   | -1.928825   |
| 32            | 6             | 0           | -2.159294  | 1.679054   | -1.366492   |
| 33            | 6             | 0           | -2.408480  | 0.791545   | -2.411541   |
| 34            | 6             | 0           | -3.717268  | 0.399021   | -2.702651   |
| 35            | 8             | 0           | -1.172007  | -2.025902  | -0.762875   |
| 36            | 8             | 0           | -1.449286  | 0.232363   | -3.207296   |
| 37            | 1             | 0           | -9.471338  | -4.244333  | -0.953608   |
| 38            | 1             | 0           | -11.942919 | -4.312634  | -0.933119   |
| 39            | 1             | 0           | -13.225549 | -2.370795  | -0.052692   |
| 40            | 1             | 0           | -12.019153 | -0.382601  | 0.786897    |
| 41            | 1             | 0           | -10.491209 | 2.316285   | 3.071079    |
| 42            | 1             | 0           | -10.005087 | 4.452420   | 4.216560    |
| 43            | 1             | 0           | -7.873191  | 5.647759   | 3.744408    |
| 44            | 1             | 0           | -6.264326  | 4.694588   | 2.128141    |
| 45            | 1             | 0           | -3.031068  | 2.808057   | 0.229758    |
| 46            | 1             | 0           | -5.778403  | 0.521135   | -2.141222   |
| 47            | 1             | 0           | -1.153200  | 1.999286   | -1.121039   |
| 48            | 1             | 0           | -3.884588  | -0.283289  | -3.528403   |
| 49            | 6             | 0           | -0.089484  | 0.597351   | -3.050923   |
|   |   |   |         |         |         |
|---|---|---|--------|--------|--------|
|50 | 6  | 0  | -0.531790 | -2.371040 | -1.982471 |
|51 | 1  | 0  | 0.009408  | 1.678998  | -2.925647 |
|52 | 1  | 0  | 0.396891  | 0.317102  | -3.988037 |
|53 | 1  | 0  | -0.329561 | -3.447138 | -2.018919 |
|54 | 1  | 0  | -1.153721 | -2.091552 | -2.836090 |
|55 | 6  | 0  | 0.620125  | -0.100255 | -1.883608 |
|56 | 6  | 0  | 0.780613  | -1.613717 | -2.041038 |
|57 | 1  | 0  | 0.123701  | 0.112447  | -0.937668 |
|58 | 6  | 0  | 0.123701  | 0.112447  | -0.937668 |
|59 | 8  | 0  | 1.582399  | -2.074155 | -0.946325 |
|60 | 6  | 0  | 3.544492  | -2.881191 | 0.053158  |
|61 | 6  | 0  | 4.944761  | -3.087607 | 0.111984  |
|62 | 6  | 0  | 2.759480  | -3.099448 | 1.191143  |
|63 | 6  | 0  | 3.315913  | -3.521092 | 2.381537  |
|64 | 6  | 0  | 4.692596  | -3.731567 | 2.485987  |
|65 | 6  | 0  | 5.515256  | -3.510499 | 1.349896  |
|66 | 6  | 0  | 5.838570  | -2.879111 | -1.000680 |
|67 | 6  | 0  | 6.925312  | -3.719175 | 1.463121  |
|68 | 6  | 0  | 7.771367  | -3.502275 | 0.347422  |
|69 | 6  | 0  | 7.172712  | -3.074773 | -0.882826 |
|70 | 6  | 0  | 5.290944  | -4.164152 | 3.719037  |
|71 | 6  | 0  | 6.624244  | -4.361168 | 3.819126  |
|72 | 6  | 0  | 7.491597  | -4.446266 | 2.694300  |
|73 | 6  | 0  | 8.872327  | -4.341413 | 2.781632  |
|74 | 6  | 0  | 9.692774  | -4.125689 | 1.681522  |
|75 | 6  | 0  | 9.148172  | -3.709805 | 0.474430  |
|76 | 1  | 0  | 1.691741  | -2.936182 | 1.127759  |
|77 | 1  | 0  | 2.683174  | -3.689653 | 3.247284  |
|78 | 1  | 0  | 5.416957  | -2.572708 | -1.945657 |
|79 | 1  | 0  | 7.820607  | -2.911484 | -1.739545 |
|80 | 1  | 0  | 4.640488  | -4.327762 | 4.572834  |
|81 | 1  | 0  | 7.066233  | -4.687242 | 4.756025  |
|82 | 1  | 0  | 9.300046  | -4.667040 | 3.725345  |
|83 | 1  | 0  | 10.763096 | -4.283227 | 1.766554  |
|84 | 1  | 0  | 9.789491  | -3.541650 | -0.385829 |
|85 | 6  | 0  | 2.859091  | -2.440642 | -1.190872 |
|86 | 8  | 0  | 3.339178  | -2.401809 | -2.306151 |
|87 | 8  | 0  | 1.952553  | 0.429725  | -1.843750 |
|88 | 6  | 0  | 2.149740  | 1.554678  | -1.121272 |
|89 | 8  | 0  | 1.221440  | 2.148451  | -0.607751 |
|90 | 6  | 0  | 3.586783  | 1.921924  | -1.047841 |
|91 | 6  | 0  | 4.019449  | 3.178764  | -0.557216 |
|92 | 6  | 0  | 4.528674  | 0.971235  | -1.458449 |
|93 | 6  | 0  | 5.421362  | 3.431414  | -0.487746 |
|94 | 6  | 0  | 3.127376  | 4.233136  | -0.138822 |
|95 | 6  | 0  | 5.884070  | 1.218498  | -1.378096 |
|96 | 1  | 0  | 4.184217  | 0.019827  | -1.842010 |
|97 | 6  | 0  | 5.908000  | 4.685891  | -0.004066 |
|98 | 6  | 0  | 6.355362  | 2.440929  | -0.894430 |
|99 | 6  | 0  | 3.596262  | 5.418144  | 0.311604  |
|100| 1  | 0  | 2.064401  | 4.051874  | -0.187557 |
|101| 1  | 0  | 6.592426  | 0.455402  | -1.685446 |
|102| 6  | 0  | 4.999733  | 5.694481  | 0.402419  |
|103| 6  | 0  | 7.304488  | 4.933529  | 0.073226  |
|104| 6  | 0  | 7.762952  | 2.716244  | -0.802981 |
105  1  0  2.899416  6.193467  0.617314
106  6  0  5.490485  6.916451  0.872487
107  6  0  7.756031  6.167280  0.549238
108  6  0  8.215864  3.903277  0.342006
109  1  0  8.456520  1.941909 -0.116290
110  6  0  6.856816  7.149546  0.944970
111  1  0  4.787508  7.684357  1.181857
112  1  0  8.824822  6.351452  0.606826
113  1  0  9.281854  4.100909 -0.277534
114  1  0  7.224502  8.102249  1.312179

SCF Done:  E(RCAM-B3LYP) =  -3065.01042328
Full mass-weighted force constant matrix:
  Low frequencies ---  -1.9236 -0.0031 -0.0021  0.0014  1.0802
2.4235
  Low frequencies ---  6.2288  8.0426  9.7118

S80
$\text{p-(P,S)-3:Ag : conformer c}$

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 1.912383  | 1.139943  | 1.983108  |
| 2             | 6             | 0           | 3.153887  | 1.739320  | 1.811645  |
| 3             | 6             | 0           | 1.836499  | -0.247193 | 2.105578  |
| 4             | 6             | 0           | 3.002254  | -1.016420 | 2.088789  |
| 5             | 6             | 0           | 4.232116  | -0.411972 | 1.913158  |
| 6             | 6             | 0           | 4.326631  | 0.979357  | 1.757497  |
| 7             | 1             | 0           | 1.022602  | 1.757785  | 1.981878  |
| 8             | 1             | 0           | 3.212111  | 2.816307  | 1.695897  |
| 9             | 1             | 0           | 2.916992  | -2.092756 | 1.920827  |
| 10            | 1             | 0           | 5.131772  | -1.015943 | 1.869068  |
| 11            | 6             | 0           | 5.583743  | 1.606914  | 1.502325  |
| 12            | 6             | 0           | 6.635776  | 2.149206  | 1.253027  |
| 13            | 6             | 0           | 7.844197  | 2.859259  | 0.984987  |
| 14            | 6             | 0           | 7.904080  | 4.232920  | 1.255456  |
| 15            | 6             | 0           | 8.983557  | 2.214804  | 0.453917  |
| 16            | 6             | 0           | 9.060058  | 4.958426  | 1.014361  |
| 17            | 6             | 0           | 10.185658 | 4.321579  | 0.497198  |
| 18            | 6             | 0           | 10.144782 | 2.963958  | 0.221515  |
| 19            | 6             | 0           | 8.994237  | 0.819082  | 0.147259  |
| 20            | 6             | 0           | 9.099314  | -0.349754 | -0.145552 |
| 21            | 6             | 0           | 9.338691  | -1.724478 | -0.453995 |
| 22            | 6             | 0           | 10.620536 | -2.248322 | -0.239302 |
| 23            | 6             | 0           | 10.905358 | -3.575757 | -0.517761 |
| 24            | 6             | 0           | 9.908131  | -4.408309 | -1.020105 |
| 25            | 6             | 0           | 8.635538  | -3.906886 | -1.243460 |
| 26            | 6             | 0           | 8.328913  | -2.567184 | -0.969728 |
| 27            | 6             | 0           | 7.007433  | -2.090042 | -1.219792 |
| 28            | 6             | 0           | 5.871361  | -1.747473 | -1.454261 |
| 29            | 6             | 0           | 4.520941  | -1.349085 | -1.693393 |
| 30            | 6             | 0           | 3.495445  | -2.299243 | -1.732078 |
| 31            | 6             | 0           | 4.186911  | 0.004953  | -1.849178 |
| 32            | 6             | 0           | 2.167765  | -1.922056 | -1.889161 |
| 33            | 6             | 0           | 1.853396  | -0.569160 | -2.013536 |
| 34            | 6             | 0           | 2.869863  | 0.388977  | -2.011082 |
| 35            | 6             | 0           | 0.673984  | -0.953110 | 2.241176  |
| 36            | 8             | 0           | 0.586098  | -0.072797 | -2.138223 |
| 37            | 1             | 0           | 7.025372  | 4.721667  | 1.661912  |
| 38            | 1             | 0           | 9.084210  | 6.021189  | 1.231745  |
| 39            | 1             | 0           | 11.094346 | 4.883314  | 0.307761  |
| 40            | 1             | 0           | 11.015806 | 2.460923  | 0.184105  |
| 41            | 1             | 0           | 11.390489 | -1.593909 | 0.154618  |
| 42            | 1             | 0           | 11.904162 | -3.961415 | -0.342235 |
| 43            | 1             | 0           | 10.123314 | -5.448864 | -1.239797 |
| 44            | 1             | 0           | 7.855450  | -4.548556 | -1.638338 |
| 45            | 1             | 0           | 3.738826  | -3.349923 | -1.615787 |
| 46            | 1             | 0           | 4.970036  | 0.754426  | -1.817082 |
| 47            | 1             | 0           | 1.396334  | -2.683237 | -1.877254 |
| 48            | 1             | 0           | 2.599734  | 1.434296  | -2.112792 |
| 49            | 6             | 0           | -0.527810 | -0.910452 | -1.873554 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 50 | 6 | 0 | -0.567920 | -0.318789 | 1.979802 |
| 51 | 1 | 0 | -0.487252 | -1.830614 | -2.462673 |
| 52 | 1 | 0 | -1.401751 | -0.335656 | -2.184125 |
| 53 | 0 | 0 | -1.330787 | -1.033833 | 2.291217 |
| 54 | 1 | 0 | -0.684278 | 0.594303 | 2.570189 |
| 55 | 6 | 0 | -0.626290 | -1.241955 | -0.383134 |
| 56 | 6 | 0 | -0.726688 | -0.007013 | 0.490570 |
| 57 | 1 | 0 | 0.253495 | -1.803368 | -0.067100 |
| 58 | 1 | 0 | 0.048877 | 0.689383 | 0.171104 |
| 59 | 8 | 0 | -2.006355 | 0.600076 | 0.274398 |
| 60 | 6 | 0 | -3.469223 | 2.440813 | 0.288570 |
| 61 | 6 | 0 | -3.713727 | 3.801823 | 0.004264 |
| 62 | 6 | 0 | -4.526755 | 1.536118 | 0.427365 |
| 63 | 6 | 0 | -5.840683 | 1.945458 | 0.311259 |
| 64 | 6 | 0 | -6.147054 | 3.279533 | 0.031079 |
| 65 | 6 | 0 | -5.089253 | 4.213814 | -0.131606 |
| 66 | 6 | 0 | -2.703276 | 4.792911 | -0.187392 |
| 67 | 6 | 0 | -5.403554 | 5.575928 | -0.429703 |
| 68 | 6 | 0 | -4.365945 | 6.525144 | -0.604022 |
| 69 | 6 | 0 | -3.009079 | 6.078777 | -0.476436 |
| 70 | 6 | 0 | -7.507365 | 3.725365 | -0.097688 |
| 71 | 6 | 0 | -7.798062 | 5.015645 | -0.376697 |
| 72 | 6 | 0 | -6.756416 | 5.989279 | -0.554995 |
| 73 | 6 | 0 | -7.039287 | 7.326371 | -0.846519 |
| 74 | 6 | 0 | -6.014833 | 8.249250 | -1.015488 |
| 75 | 6 | 0 | -4.689598 | 7.853442 | -0.895950 |
| 76 | 1 | 0 | -4.306568 | 0.498647 | 0.644877 |
| 77 | 1 | 0 | -6.646494 | 1.229919 | 0.443618 |
| 78 | 1 | 0 | -1.671281 | 4.490138 | -0.090145 |
| 79 | 1 | 0 | -2.213995 | 6.805059 | -0.619010 |
| 80 | 1 | 0 | -8.299985 | 2.995225 | 0.034562 |
| 81 | 1 | 0 | -8.829796 | 5.340979 | -0.472526 |
| 82 | 1 | 0 | -8.075291 | 7.638456 | -0.940195 |
| 83 | 1 | 0 | -6.251813 | 9.283748 | -1.241921 |
| 84 | 1 | 0 | -3.889306 | 8.575518 | -1.028858 |
| 85 | 6 | 0 | -2.087696 | 1.934349 | 0.483077 |
| 86 | 8 | 0 | -1.119222 | 2.590639 | 0.808912 |
| 87 | 8 | 0 | -1.789971 | -2.048704 | -0.152296 |
| 88 | 6 | 0 | -1.669391 | -3.732340 | -0.376720 |
| 89 | 8 | 0 | -0.629409 | -3.872518 | -0.753844 |
| 90 | 6 | 0 | -2.892626 | -4.158904 | -0.062814 |
| 91 | 6 | 0 | -4.221340 | -3.678730 | -0.118676 |
| 92 | 6 | 0 | -2.638985 | -5.483037 | 0.304805 |
| 93 | 6 | 0 | -5.274188 | -4.572847 | 0.239107 |
| 94 | 6 | 0 | -4.585854 | -2.355325 | -0.559785 |
| 95 | 6 | 0 | -3.659460 | -6.340143 | 0.663447 |
| 96 | 1 | 0 | -1.610380 | -5.823574 | 0.315279 |
| 97 | 6 | 0 | -6.637079 | -4.141545 | 0.193269 |
| 98 | 6 | 0 | -4.986330 | -5.904199 | 0.644231 |
| 99 | 6 | 0 | -5.881349 | -1.959720 | -0.613329 |
| 100 | 1 | 0 | -3.809803 | -1.667161 | -0.852394 |
| 101 | 1 | 0 | -3.436117 | -7.359144 | 0.963453 |
| 102 | 6 | 0 | -6.956318 | -2.827517 | -0.230148 |
| 103 | 6 | 0 | -7.683688 | -5.026106 | 0.567088 |
| 104 | 6 | 0 | -6.064839 | -6.778035 | 1.017807 |
105    1    0      -6.125190   -0.959316   -0.959606
106    6    0      -8.292808   -2.419865   -0.269464
107    6    0      -9.007286   -4.580426    0.517621
108    6    0      -7.349432   -6.359892    0.984230
109    1    0      -5.818829   -7.788904    1.328389
110    6    0      -9.308624   -3.289257    0.103481
111    1    0      -8.528388   -1.411437   -0.597128
112    1    0      -9.803726   -5.259733    0.806837
113    1    0      -8.156268   -7.028774    1.268930
114    1    0      -10.342138  -2.960161    0.069769

SCF Done: E(RCAM-B3LYP) =  -3065.01026797
Full mass-weighted force constant matrix:
Low frequencies --- -2.1324   -1.8786   -0.0029   -0.0015   -0.0008
2.9417
Low frequencies ---  7.8059    9.6325   10.6263
\[ p-(P,S)-3:Ag \] : conformer \textbf{d}  

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X     | Y     | Z     |
| 1             | 6             | 0           | -2.172751 | 1.681582 | -1.359884 |
| 2             | 6             | 0           | -3.255116 | 2.121184 | -0.606756 |
| 3             | 6             | 0           | -2.392506 | 0.780454 | -2.399825 |
| 4             | 6             | 0           | -3.689776 | 0.358600 | -2.701301 |
| 5             | 6             | 0           | -4.757263 | 0.795881 | -1.942963 |
| 6             | 6             | 0           | -4.554610 | 1.676943 | -0.869787 |
| 7             | 6             | 0           | -1.175959 | 2.023576 | -1.106011 |
| 8             | 6             | 0           | -3.084620 | 2.806876 | 0.216486  |
| 9             | 6             | 0           | -3.834084 | -0.334150 | -3.522709 |
| 10            | 6             | 0           | -5.759043 | 0.444028 | -2.163374 |
| 11            | 6             | 0           | -5.639669 | 2.079749 | -0.032367 |
| 12            | 6             | 0           | -6.537846 | 2.405620 | 0.709696  |
| 13            | 6             | 0           | -7.528886 | 2.893955 | 1.613930  |
| 14            | 6             | 0           | -7.304115 | 4.119079 | 2.257662  |
| 15            | 6             | 0           | -8.721704 | 2.188190 | 1.884765  |
| 16            | 6             | 0           | -8.230548 | 4.643570 | 3.144415  |
| 17            | 6             | 0           | -9.409907 | 3.950600 | 3.406707  |
| 18            | 6             | 0           | -9.649238 | 2.737607 | 2.781612  |
| 19            | 6             | 0           | -9.035982 | 0.930065 | 1.282643  |
| 20            | 6             | 0           | -9.427321 | -0.131392 | 0.853388  |
| 21            | 6             | 0           | -10.030877 | -1.334540 | 0.371648  |
| 22            | 6             | 0           | -11.429817 | -1.423735 | 0.373248  |
| 23            | 6             | 0           | -12.074108 | -2.562420 | -0.083608 |
| 24            | 6             | 0           | -11.327482 | -3.640684 | -0.552426 |
| 25            | 6             | 0           | -9.943255 | -3.572962 | -0.557419 |
| 26            | 6             | 0           | -9.274010 | -2.430889 | -0.097762 |
| 27            | 6             | 0           | -7.847693 | -2.402321 | -0.120379 |
| 28            | 6             | 0           | -6.639791 | -2.431570 | -0.171274 |
| 29            | 6             | 0           | -5.215116 | -2.414725 | -0.268455 |
| 30            | 6             | 0           | -4.447716 | -1.642224 | 0.617797  |
| 31            | 6             | 0           | -4.559621 | -3.122796 | -1.280093 |
| 32            | 6             | 0           | -3.079911 | -1.546840 | 0.462525  |
| 33            | 6             | 0           | -2.447072 | -2.208385 | -0.592615 |
| 34            | 6             | 0           | -3.183598 | -3.027678 | -1.446099 |
| 35            | 6             | 0           | -1.413575 | 0.234910 | -3.180733 |
| 36            | 6             | 0           | -1.112319 | -1.981169 | -0.713191 |
| 37            | 6             | 0           | -6.385270 | 4.654805 | 2.045834  |
| 38            | 6             | 0           | -8.033939 | 5.593861 | 3.629823  |
| 39            | 6             | 0           | -10.141532 | 4.354737 | 4.098480  |
| 40            | 6             | 0           | -10.563599 | 2.189868 | 2.981993  |
| 41            | 6             | 0           | -12.003970 | 0.578759 | 0.737412  |
| 42            | 6             | 0           | -13.158054 | -2.608788 | -0.075125 |
| 43            | 6             | 0           | -11.824627 | -4.535420 | -0.912434 |
| 44            | 6             | 0           | -9.355188 | -4.410054 | -0.917514 |
| 45            | 6             | 0           | -4.942977 | -1.092419 | 1.410542  |
| 46            | 6             | 0           | -5.138028 | -3.739903 | -1.959428 |
| 47            | 6             | 0           | -2.482707 | -0.926205 | 1.121038  |
| 48            | 6             | 0           | -2.702735 | -3.577943 | -2.245765 |
| 49            | 6             | 0           | -0.454713 | -2.335075 | -1.920843 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 50| 6 | 0 | -0.063837| 0.631337 | -3.015093|
| 51| 1 | 0 | -1.074630| -2.082262| -2.896466|
| 52| 1 | 0 | -0.231202| -3.407409| -1.936948|
| 53| 1 | 0 | 0.436995 | 0.356104 | -3.946057|
| 54| 1 | 0 | 0.009660 | 1.715802 | -2.896466|
| 55| 6 | 0 | 0.843353 | -1.553968| -1.983560|
| 56| 6 | 0 | 0.651897 | -0.042673| -1.837406|
| 57| 1 | 0 | 1.361105 | -1.781647| -2.917649|
| 58| 1 | 0 | 0.144711 | 0.166726 | -0.896541|
| 59| 8 | 0 | 1.971898 | 0.516793 | -1.793785|
| 60| 6 | 0 | 3.563304 | 2.071418 | -1.030057|
| 61| 6 | 0 | 3.959005 | 3.337684 | -0.531341|
| 62| 6 | 0 | 4.531108 | 1.164583 | -1.479032|
| 63| 6 | 0 | 5.876816 | 1.467934 | -1.435129|
| 64| 6 | 0 | 6.312143 | 2.701499 | -0.946206|
| 65| 6 | 0 | 5.351126 | 3.646006 | -0.495842|
| 66| 6 | 0 | 3.038231 | 4.346714 | -0.069667|
| 67| 6 | 0 | 5.800963 | 4.911157 | -0.004183|
| 68| 6 | 0 | 4.865261 | 5.875137 | 0.445814|
| 69| 6 | 0 | 3.472131 | 5.543555 | 0.389326|
| 70| 6 | 0 | 7.709530 | 3.032963 | -0.891726|
| 71| 6 | 0 | 8.127630 | 4.229597 | -0.422779|
| 72| 6 | 0 | 7.188012 | 5.214339 | 0.037522|
| 73| 6 | 0 | 7.603231 | 6.457203 | 0.522843|
| 74| 6 | 0 | 6.677220 | 7.395191 | 0.961884|
| 75| 6 | 0 | 5.319880 | 7.107941 | 0.923876|
| 76| 6 | 0 | 4.216992 | 0.202635 | -1.862861|
| 77| 6 | 0 | 6.606968 | 0.742299 | -1.779662|
| 78| 6 | 0 | 1.982305 | 4.125959 | -0.928855|
| 79| 6 | 0 | 2.753798 | 6.284592 | 0.728573|
| 80| 6 | 0 | 8.424131 | 2.293061 | -1.239171|
| 81| 6 | 0 | 9.186231 | 4.469618 | -0.386082|
| 82| 6 | 0 | 8.664934 | 6.683913 | 0.553189|
| 83| 6 | 0 | 7.016836 | 8.355696 | 1.335727|
| 84| 6 | 0 | 4.595830 | 7.841287 | 1.266693|
| 85| 6 | 0 | 2.139101 | 1.653442 | -1.081702|
| 86| 6 | 0 | 1.195968 | 2.219644 | -0.563887|
| 87| 6 | 0 | 1.653256 | -1.997054 | -0.887506|
| 88| 6 | 0 | 2.953346 | -2.279801 | -1.122733|
| 89| 6 | 0 | 3.432107 | -2.223718 | -2.237999|
| 90| 6 | 0 | 3.666855 | -2.646419 | 0.129615|
| 91| 6 | 0 | 4.986525 | -3.162681 | 0.125108|
| 92| 6 | 0 | 2.996509 | -2.461630 | 1.344362|
| 93| 6 | 0 | 5.595377 | -3.476680 | 1.376364|
| 94| 6 | 0 | 5.754051 | -3.404324 | -1.071601|
| 95| 6 | 0 | 3.593165 | -2.761783 | 2.551978|
| 96| 6 | 0 | 1.987511 | -2.071816 | 1.329671|
| 97| 6 | 0 | 6.923431 | -4.004570 | 1.424138|
| 98| 6 | 0 | 4.892937 | -3.270649 | 2.593977|
| 99| 6 | 0 | 7.009438 | -3.906821 | -1.017503|
|100| 6 | 0 | 5.302540 | -3.172984 | -2.023825|
|101| 6 | 0 | 3.051915 | -2.602960 | 3.479412|
|102| 6 | 0 | 7.646927 | -4.225072 | 0.226049|
|103| 6 | 0 | 7.529752 | -4.314214 | 2.670812|
|104| 6 | 0 | 5.530191 | -3.590731 | 3.841811|
|   |   |   |   |
|---|---|---|---|
| 105| 1 | 0 | 7.561964 -4.080228 -1.936698 |
| 106| 6 | 0 | 8.944231 -4.742839  0.288249 |
| 107| 6 | 0 | 8.828388 -4.829649  2.691825 |
| 108| 6 | 0 | 6.786348 -4.087873  3.879339 |
| 109| 1 | 0 | 4.972708 -3.422582  4.758189 |
| 110| 6 | 0 | 9.528879 -5.041991  1.511026 |
| 111| 1 | 0 | 9.491544 -4.909362 -0.634993 |
| 112| 1 | 0 | 9.287361 -5.064419  3.647718 |
| 113| 1 | 0 | 7.258247 -4.327023  4.827842 |
| 114| 1 | 0 |10.536583 -5.443260  1.545321 |

SCF Done: E(RCAM-B3LYP) = -3065.01023629
Full mass-weighted force constant matrix:
  Low frequencies ---  -1.7284  -1.0486  -0.0027  -0.0011  0.0017  
            3.6020
  Low frequencies ---  5.9172   6.9658   9.6305
**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 2.983782   | 2.134880   | -2.481738   |
| 2             | 6             | 0           | 4.361692   | 2.103661   | -2.306759   |
| 3             | 6             | 0           | 2.154342   | 1.707435   | -1.447164   |
| 4             | 6             | 0           | 2.702251   | 1.321999   | -0.221743   |
| 5             | 6             | 0           | 4.072075   | 1.289473   | -0.057232   |
| 6             | 6             | 0           | 4.926835   | 1.656577   | -1.108711   |
| 7             | 1             | 0           | 2.571975   | 2.473779   | -0.571976   |
| 8             | 1             | 0           | 5.010382   | 2.410446   | -3.120348   |
| 9             | 1             | 0           | 2.034022   | 1.007178   | 0.571976    |
| 10            | 1             | 0           | 4.497358   | 0.946665   | 0.879608    |
| 11            | 6             | 0           | 6.342412   | 1.520337   | -0.976454   |
| 12            | 6             | 0           | 7.536736   | 1.354158   | -0.883809   |
| 13            | 6             | 0           | 8.955806   | 1.212777   | -0.832985   |
| 14            | 6             | 0           | 9.755113   | 2.070134   | -1.600913   |
| 15            | 6             | 0           | 9.577492   | 0.228380   | -0.033203   |
| 16            | 6             | 0           | 11.137030  | 1.967527   | -1.581573   |
| 17            | 6             | 0           | 11.750741  | 1.001091   | -0.788362   |
| 18            | 6             | 0           | 10.976679  | 0.143156   | -0.023404   |
| 19            | 6             | 0           | 8.836678   | -0.688248  | 0.776079    |
| 20            | 6             | 0           | 8.322872   | -1.513068  | 1.497030    |
| 21            | 6             | 0           | 7.857519   | -2.479945  | 2.441914    |
| 22            | 6             | 0           | 8.713835   | -2.840077  | 3.492317    |
| 23            | 6             | 0           | 8.326637   | -3.766619  | 4.446802    |
| 24            | 6             | 0           | 7.067176   | -4.356129  | 4.368572    |
| 25            | 6             | 0           | 6.208809   | -4.016707  | 3.335250    |
| 26            | 6             | 0           | 6.583133   | -3.083006  | 2.358722    |
| 27            | 6             | 0           | 5.658789   | -2.775707  | 1.315289    |
| 28            | 6             | 0           | 4.810485   | -2.580737  | 0.475212    |
| 29            | 6             | 0           | 3.794297   | -2.316647  | -0.493228   |
| 30            | 6             | 0           | 2.447267   | -2.533000  | 0.187111    |
| 31            | 6             | 0           | 4.119587   | -1.792367  | -1.753635   |
| 32            | 6             | 0           | 1.438646   | -2.205972  | 1.068229    |
| 33            | 6             | 0           | 1.782663   | -1.651822  | -2.317557   |
| 34            | 6             | 0           | 3.125799   | -1.470018  | -2.655701   |
| 35            | 8             | 0           | 0.799665   | 1.619186   | -1.539367   |
| 36            | 8             | 0           | 0.890141   | -1.236650  | -3.264809   |
| 37            | 1             | 0           | 9.270324   | 2.822474   | -2.213418   |
| 38            | 1             | 0           | 11.736108  | 2.642596   | -2.183812   |
| 39            | 1             | 0           | 12.832121  | 0.915615   | -0.766843   |
| 40            | 1             | 0           | 11.446769  | -0.613705  | 0.594992    |
| 41            | 1             | 0           | 9.691579   | -2.373915  | 3.547225    |
| 42            | 1             | 0           | 9.005694   | -4.027949  | 5.251627    |
| 43            | 1             | 0           | 6.754938   | -5.082070  | 5.112103    |
| 44            | 1             | 0           | 5.228132   | -4.474508  | 3.265713    |
| 45            | 1             | 0           | 2.181504   | -2.944167  | 0.781010    |
| 46            | 1             | 0           | 5.159679   | -1.621973  | -2.008698   |
| 47            | 1             | 0           | 0.404192   | -2.360577  | 0.801583    |
| 48            | 1             | 0           | 3.366133   | -1.048384  | -3.625081   |
| 49            | 6             | 0           | -0.499336  | -1.429276  | -3.071106   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 50 | 6 | 0 | 0.184510 | 1.662364 | -2.818851 |
| 51 | 1 | 0 | -0.700158 | -2.429743 | -2.678045 |
| 52 | 1 | 0 | -0.944740 | -1.358648 | -3.157072 |
| 53 | 1 | 0 | 0.076608  | 2.698695  | -3.548406 |
| 54 | 1 | 0 | 0.774313  | 1.102945  | -3.548406 |
| 55 | 6 | 0 | -1.160427 | -0.398643 | -2.146758 |
| 56 | 6 | 0 | -1.187597 | 1.030975  | -2.687018 |
| 57 | 1 | 0 | -0.701439 | -0.402359 | -1.158887 |
| 58 | 1 | 0 | -1.699826 | 1.061084  | -3.650612 |
| 59 | 8 | 0 | -1.926879 | 1.821975  | -2.687018 |
| 60 | 6 | 0 | -3.833694 | 3.065630  | -1.031673 |
| 61 | 6 | 0 | -3.228998 | 3.679175  | 0.094007  |
| 62 | 6 | 0 | -5.210465 | 3.194670  | -1.241102 |
| 63 | 6 | 0 | -6.018323 | 3.887160  | -0.364493 |
| 64 | 6 | 0 | -5.469269 | 4.499702  | 0.763675  |
| 65 | 6 | 0 | -4.069941 | 4.404850  | 0.993836  |
| 66 | 6 | 0 | -1.815496 | 3.648144  | 0.386829  |
| 67 | 6 | 0 | -3.517127 | 5.051797  | 2.144299  |
| 68 | 6 | 0 | -2.125036 | 4.988821  | 2.399025  |
| 69 | 6 | 0 | -1.302121 | 4.267668  | 1.474549  |
| 70 | 6 | 0 | -6.294427 | 5.226200  | 1.689289  |
| 71 | 6 | 0 | -5.765049 | 5.829099  | 2.776317  |
| 72 | 6 | 0 | -4.355008 | 5.765599  | 3.042782  |
| 73 | 6 | 0 | -3.790913 | 6.387959  | 4.159603  |
| 74 | 6 | 0 | -2.424469 | 6.318378  | 4.399258  |
| 75 | 6 | 0 | -1.597436 | 5.625454  | 3.526354  |
| 76 | 1 | 0 | -5.635643 | 2.725795  | -2.119982 |
| 77 | 1 | 0 | -7.086018 | 3.960278  | -0.546393 |
| 78 | 1 | 0 | -1.152756 | 3.111217  | -0.273495 |
| 79 | 1 | 0 | -0.233304 | 4.224115  | 1.663970  |
| 80 | 1 | 0 | -7.360386 | 5.278540  | 1.489647  |
| 81 | 1 | 0 | -6.397568 | 6.375958  | 3.469402  |
| 82 | 1 | 0 | -4.437369 | 6.930990  | 4.842807  |
| 83 | 1 | 0 | -2.002907 | 6.807867  | 5.271246  |
| 84 | 1 | 0 | -0.528664 | 5.571162  | 3.711678  |
| 85 | 6 | 0 | -3.148790 | 2.265026  | -2.087064 |
| 86 | 8 | 0 | -3.660236 | 2.005658  | -3.158028 |
| 87 | 8 | 0 | -2.535311 | -0.788787 | -2.031161 |
| 88 | 6 | 0 | -2.852945 | -1.672858 | -1.059805 |
| 89 | 8 | 0 | -1.998253 | -2.172263 | -0.354211 |
| 90 | 6 | 0 | -4.316086 | -1.919840 | -0.975728 |
| 91 | 6 | 0 | -4.870737 | -2.972215 | -0.227707 |
| 92 | 6 | 0 | -5.156607 | -1.069516 | -1.726462 |
| 93 | 6 | 0 | -6.288256 | -3.129872 | -0.219214 |
| 94 | 6 | 0 | -4.088165 | -3.909741 | 0.538798  |
| 95 | 6 | 0 | -6.527955 | -1.223940 | -1.706840 |
| 96 | 1 | 0 | -4.719476 | -0.271948 | -2.313604 |
| 97 | 6 | 0 | -6.895904 | -4.180476 | 0.536751  |
| 98 | 6 | 0 | -7.117897 | -2.246793 | -0.960867 |
| 99 | 6 | 0 | -4.671172 | -4.903307 | 1.248896  |
| 100| 1 | 0  | -3.014609 | -3.800743 | 0.539823  |
| 101| 1 | 0  | -7.158224 | -0.546585 | -2.274686 |
| 102| 6 | 0  | -6.093172 | -5.079627 | 1.281339  |
| 103| 6 | 0  | -8.307897 | -4.334040 | 0.547915  |
| 104| 6 | 0  | -8.543819 | -2.423773 | -0.931607 |
|   |   |   |                |                |                |
|---|---|---|----------------|----------------|----------------|
| 105| 1 | 0 | -4.054914      | -5.595217      | 1.816061       |
| 106| 6 | 0 | -6.701554      | -6.102479      | 2.015234       |
| 107| 6 | 0 | -8.878641      | -5.368305      | 1.294408       |
| 108| 6 | 0 | -9.111508      | -3.417645      | -0.212774      |
| 109| 1 | 0 | -9.156173      | -1.735349      | -1.506020      |
| 110| 6 | 0 | -8.082275      | -6.244372      | 2.021207       |
| 111| 1 | 0 | -6.078914      | -6.787845      | 2.582842       |
| 112| 1 | 0 | -9.958853      | -5.480804      | 1.300206       |
| 113| 1 | 0 | -10.190241     | -3.542674      | -0.198004      |
| 114| 1 | 0 | -8.541714      | -7.042424      | 2.595362       |

SCF Done:  $E_{(RCAM-B3LYP)} = -3065.00901017$

Full mass-weighted force constant matrix:

- Low frequencies --- -2.4485 -0.0033 -0.0016 -0.0007 1.6395 4.0336
- Low frequencies --- 7.2066 7.5689 9.9578
$p$-$(P,S)$-3:Ag  conformer a

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 1.031405   | 1.312813  | 1.999968  |
| 2             | 6             | 0           | 2.384810   | 1.620183  | 1.959390  |
| 3             | 6             | 0           | 0.635484   | 0.001271  | 2.273398  |
| 4             | 6             | 0           | 1.595616   | -0.982671 | 2.537469  |
| 5             | 6             | 0           | 2.937747   | -0.670115 | 2.497738  |
| 6             | 6             | 0           | 3.525625   | 0.637851  | 2.194341  |
| 7             | 1             | 0           | 0.305600   | 2.091793  | 1.797409  |
| 8             | 1             | 0           | 2.694570   | 2.634458  | 1.732120  |
| 9             | 1             | 0           | 1.259609   | -1.989181 | 2.759236  |
| 10            | 1             | 0           | 3.679384   | -1.437339 | 2.692825  |
| 11            | 6             | 0           | 4.748554   | 0.948050  | 2.115644  |
| 12            | 6             | 0           | 5.945558   | 1.202243  | 2.078287  |
| 13            | 6             | 0           | 7.284673   | 1.638446  | 2.379666  |
| 14            | 6             | 0           | 7.473058   | 2.491995  | 3.471767  |
| 15            | 6             | 0           | 8.406189   | 1.224367  | 1.626388  |
| 16            | 6             | 0           | 8.743001   | 2.929191  | 3.818128  |
| 17            | 6             | 0           | 9.848443   | 2.516607  | 3.079240  |
| 18            | 6             | 0           | 9.681568   | 1.670843  | 1.993434  |
| 19            | 6             | 0           | 8.288405   | 0.360381  | 0.490808  |
| 20            | 6             | 0           | 8.288437   | -0.360295 | -0.490824 |
| 21            | 6             | 0           | 8.406200   | -1.224345 | -1.626362 |
| 22            | 6             | 0           | 9.681579   | -1.670843 | -1.993372 |
| 23            | 6             | 0           | 9.848482   | -2.516630 | -3.079160 |
| 24            | 6             | 0           | 8.743061   | -2.929200 | -3.818080 |
| 25            | 6             | 0           | 7.473110   | -2.491997 | -3.471742 |
| 26            | 6             | 0           | 7.284700   | -1.638443 | -2.379652 |
| 27            | 6             | 0           | 5.945567   | -1.202289 | -2.078283 |
| 28            | 6             | 0           | 4.748552   | -0.948150 | -2.115638 |
| 29            | 6             | 0           | 3.352561   | -0.637950 | -2.194368 |
| 30            | 6             | 0           | 2.384803   | -1.620254 | -1.959320 |
| 31            | 6             | 0           | 2.937761   | 0.669992  | -2.497874 |
| 32            | 6             | 0           | 1.031401   | -1.312875 | -1.999909 |
| 33            | 6             | 0           | 0.635494   | -0.001348 | -2.273437 |
| 34            | 6             | 0           | 1.595630   | 0.982559  | -2.537612 |
| 35            | 8             | 0           | -0.649199  | -0.432440 | 2.305281  |
| 36            | 8             | 0           | -0.649185  | 0.432378  | -2.305323 |
| 37            | 1             | 0           | 6.609362   | 2.806575  | 4.046352  |
| 38            | 1             | 0           | 8.869169   | 3.591393  | 4.667658  |
| 39            | 1             | 0           | 10.842987  | 2.855450  | 3.348026  |
| 40            | 1             | 0           | 10.538523  | 1.348266  | 1.413141  |
| 41            | 1             | 0           | 10.538523  | -1.348269 | -1.413060 |
| 42            | 1             | 0           | 10.843030  | -2.855503 | -3.347894 |
| 43            | 1             | 0           | 8.869246   | -3.591389 | -4.667617 |
| 44            | 1             | 0           | 6.609426   | -2.806574 | -4.046345 |
| 45            | 1             | 0           | 2.694557   | -2.634512 | -1.731963 |
| 46            | 1             | 0           | 3.679406   | 1.437187  | -2.693043 |
| 47            | 1             | 0           | 0.305587   | -2.091834 | -1.797298 |
| 48            | 1             | 0           | 1.259630   | 1.989053  | -2.759462 |
| 49            | 6             | 0           | -1.707421  | -0.427364 | -1.908083 |
|   |   |   |     |     |     |
|---|---|---|-----|-----|-----|
| 50 | 6 | 0 | -1.707418 | 0.427322 | 1.908060 |
| 51 | 1 | 0 | -1.655154 | -1.388083 | -2.426735 |
| 52 | 1 | 0 | -2.621284 | 0.084949 | 2.209239 |
| 53 | 1 | 0 | -2.621296 | -0.084988 | 2.209293 |
| 54 | 1 | 0 | -1.655152 | 1.388025 | 2.426737 |
| 55 | 6 | 0 | -1.720478 | -0.647491 | -0.393970 |
| 56 | 6 | 0 | -1.720460 | 0.647483 | 0.393947 |
| 57 | 1 | 0 | -0.845191 | -1.220085 | -0.086606 |
| 58 | 1 | 0 | -0.845152 | 1.220051 | 0.086589 |
| 59 | 8 | 0 | -2.893072 | 1.392270 | 0.057519 |
| 60 | 6 | 0 | -4.046770 | 3.417006 | -0.283848 |
| 61 | 6 | 0 | -4.228986 | 4.818354 | -0.167387 |
| 62 | 6 | 0 | -5.063105 | 2.625965 | -0.834754 |
| 63 | 6 | 0 | -6.246910 | 3.177391 | -1.279780 |
| 64 | 6 | 0 | -6.467511 | 4.554033 | -1.186816 |
| 65 | 6 | 0 | -5.457406 | 5.381245 | -0.625783 |
| 66 | 6 | 0 | -3.250678 | 5.715489 | 0.395875 |
| 67 | 6 | 0 | -5.691042 | 6.788531 | -0.527314 |
| 68 | 6 | 0 | -4.704289 | 7.638323 | 0.031166 |
| 69 | 6 | 0 | -3.481478 | 7.046300 | 0.487617 |
| 70 | 6 | 0 | -7.694235 | 5.145824 | -1.645375 |
| 71 | 6 | 0 | -7.907129 | 6.477591 | -1.550567 |
| 72 | 6 | 0 | -6.913138 | 7.348410 | -0.986636 |
| 73 | 6 | 0 | -7.118774 | 8.726736 | -0.879349 |
| 74 | 6 | 0 | -6.144410 | 9.551075 | -0.329840 |
| 75 | 6 | 0 | -4.947162 | 9.012601 | 0.121841 |
| 76 | 1 | 0 | -4.911650 | 1.557614 | -0.912140 |
| 77 | 1 | 0 | -7.016086 | 2.541285 | -1.706168 |
| 78 | 1 | 0 | -2.317761 | 5.301583 | 0.745480 |
| 79 | 1 | 0 | -2.725444 | 7.696818 | 0.918251 |
| 80 | 1 | 0 | -8.449366 | 4.492505 | -2.071557 |
| 81 | 1 | 0 | -8.837745 | 6.914913 | -1.900016 |
| 82 | 1 | 0 | -8.054790 | 9.149496 | -1.232255 |
| 83 | 1 | 0 | -6.320399 | 10.619115 | -0.253810 |
| 84 | 1 | 0 | -4.185580 | 9.656721 | 0.551373 |
| 85 | 6 | 0 | -2.801803 | 2.741072 | 0.156562 |
| 86 | 8 | 0 | -1.786203 | 3.269511 | 0.566386 |
| 87 | 8 | 0 | -2.893116 | -1.392234 | -0.057543 |
| 88 | 6 | 0 | -2.801899 | -2.741038 | -0.156580 |
| 89 | 8 | 0 | -1.786308 | -3.269526 | -0.566365 |
| 90 | 6 | 0 | -4.046882 | -3.416938 | -0.283830 |
| 91 | 6 | 0 | -4.229103 | -4.818279 | 0.167356 |
| 92 | 6 | 0 | -5.063204 | -2.625900 | 0.834765 |
| 93 | 6 | 0 | -5.457504 | -5.381178 | 0.625786 |
| 94 | 6 | 0 | -3.250816 | -5.715392 | -0.395879 |
| 95 | 6 | 0 | -6.246998 | -3.177331 | 1.279820 |
| 96 | 1 | 0 | -4.911747 | -1.557550 | 0.912155 |
| 97 | 6 | 0 | -5.691135 | -6.788463 | 0.527309 |
| 98 | 6 | 0 | -6.467593 | -4.553975 | 1.186862 |
| 99 | 6 | 0 | -3.481615 | -7.046203 | -0.487728 |
| 100 | 1 | 0 | -2.317916 | -5.301471 | -0.745608 |
| 101 | 1 | 0 | -7.016170 | -2.541230 | 1.706223 |
| 102 | 6 | 0 | -4.704400 | -7.638241 | -0.031226 |
| 103 | 6 | 0 | -6.913207 | -7.348355 | 0.986680 |
| 104 | 6 | 0 | -7.694290 | -5.145780 | 1.645473 |
|   |   |   |          |          |          |
|---|---|---|---------|---------|---------|
| 105| 1 | 0 | -2.725601| -7.696705| -0.918421|
| 106| 6 | 0 | -4.947267| -9.012520| -0.121905|
| 107| 6 | 0 | -7.118838| -8.726681|  0.879385|
| 108| 6 | 0 | -7.907177| -6.477548|  1.550666|
| 109| 1 | 0 | -8.449405| -4.492472|  2.071702|
| 110| 6 | 0 | -6.144491| -9.551007|  0.329823|
| 111| 1 | 0 | -4.185699| -9.656630| -0.551477|
| 112| 1 | 0 | -8.054835| -9.149452|  1.232327|
| 113| 1 | 0 | -8.837773| -6.914879|  1.900161|
| 114| 1 | 0 | -6.320477| -10.619048|  0.253789|
| 115| 47| 0 |  5.752668| -0.000052|  0.000014|

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SCF Done: \( E(\text{RCAM-B3LYP}) = -3210.52772521 \) A.U. after 18 cycles

Full mass-weighted force constant matrix:

Low frequencies --- -0.0014 -0.0013 -0.0008  1.3328  3.1783  4.1108

Low frequencies ---  6.7091  8.5754  9.8111
### Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 1.282210    | 0.832373    | 2.103443    |
| 2             | 6             | 0           | 2.605162    | 1.254079    | 2.079486    |
| 3             | 6             | 0           | 0.999003    | -0.521999   | 2.294117    |
| 4             | 6             | 0           | 2.039403    | -1.436344   | 2.497207    |
| 5             | 6             | 0           | 3.350232    | -1.010443   | 2.476064    |
| 6             | 6             | 0           | 3.653004    | 0.343611    | 2.251546    |
| 7             | 1             | 0           | 0.492691    | 1.559051    | 1.951386    |
| 8             | 1             | 0           | 2.827049    | 2.302641    | 1.913600    |
| 9             | 1             | 0           | 1.790183    | -2.479152   | 2.657056    |
| 10            | 1             | 0           | 4.154869    | -1.723059   | 2.622689    |
| 11            | 6             | 0           | 5.018159    | 0.770492    | 2.180496    |
| 12            | 6             | 0           | 6.191037    | 1.118928    | 2.141813    |
| 13            | 6             | 0           | 7.491368    | 1.661416    | 2.439799    |
| 14            | 6             | 0           | 7.616994    | 2.510022    | 3.544773    |
| 15            | 6             | 0           | 8.636317    | 1.358123    | 1.669154    |
| 16            | 6             | 0           | 8.848070    | 3.049352    | 3.887175    |
| 17            | 6             | 0           | 9.777211    | 2.745327    | 3.131645    |
| 18            | 6             | 0           | 9.872384    | 1.906460    | 2.032821    |
| 19            | 6             | 0           | 8.582319    | 0.506428    | 0.519138    |
| 20            | 6             | 0           | 8.640118    | -0.198339   | -0.472566   |
| 21            | 6             | 0           | 8.825799    | -1.027114   | -1.625485   |
| 22            | 6             | 0           | 10.131801   | -1.369162   | -1.994678   |
| 23            | 6             | 0           | 10.364304   | -2.175375   | -3.100291   |
| 24            | 6             | 0           | 9.294922    | -2.652402   | -3.853193   |
| 25            | 6             | 0           | 7.994837    | -2.318707   | -3.503246   |
| 26            | 6             | 0           | 7.740458    | -1.506247   | -2.393439   |
| 27            | 6             | 0           | 6.373153    | -1.174977   | -2.088680   |
| 28            | 6             | 0           | 5.163139    | -0.992522   | -2.107484   |
| 29            | 6             | 0           | 3.751646    | -0.754799   | -2.169021   |
| 30            | 6             | 0           | 2.838550    | -1.801216   | -2.004025   |
| 31            | 6             | 0           | 3.267517    | 0.546922    | -2.383588   |
| 32            | 6             | 0           | 1.470469    | -1.564847   | -2.027330   |
| 33            | 6             | 0           | 1.005115    | -0.260772   | -2.211735   |
| 34            | 6             | 0           | 1.910472    | 0.789219    | -2.404584   |
| 35            | 8             | 0           | -0.244345   | -1.064491   | 2.296966    |
| 36            | 8             | 0           | -0.301500   | 0.104872    | -2.217684   |
| 37            | 1             | 0           | 6.735462    | 2.739402    | 4.132466    |
| 38            | 1             | 0           | 8.925549    | 3.706130    | 4.746999    |
| 39            | 1             | 0           | 10.941668   | 3.163980    | 3.397504    |
| 40            | 1             | 0           | 10.747876   | 1.668906    | 1.439372    |
| 41            | 1             | 0           | 10.960712   | -0.996764   | -1.405477   |
| 42            | 1             | 0           | 11.382115   | -2.432987   | -3.372010   |
| 43            | 1             | 0           | 9.472580    | -3.284212   | -4.716551   |
| 44            | 1             | 0           | 7.158607    | -2.683665   | -4.088573   |
| 45            | 1             | 0           | 3.202383    | -2.810485   | -1.845321   |
| 46            | 1             | 0           | 3.967126    | 1.364031    | -2.523654   |
| 47            | 1             | 0           | 0.787952    | -2.394025   | -1.881316   |
| 48            | 1             | 0           | 1.520658    | 1.789042    | -2.558065   |
| 49            | 6             | 0           | -1.312815   | -0.839978   | -1.901460   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|50 | 6 | 0 | -1.376227 | -0.273691 | 1.967369 |
|51 | 1 | 0 | -1.202516 | -1.752838 | -2.492452 |
|52 | 1 | 0 | -2.251383 | -0.356179 | -2.173267 |
|53 | 1 | 0 | -2.239627 | -0.883066 | 2.234999 |
|54 | 1 | 0 | -1.400777 | 0.648845 | 2.554044 |
|55 | 6 | 0 | -1.323545 | -1.175452 | -0.408377 |
|56 | 6 | 0 | -1.430031 | 0.052044 | 0.473013 |
|57 | 1 | 0 | -0.413251 | -1.706719 | -0.130419 |
|58 | 1 | 0 | -0.619267 | 0.726379 | 0.197432 |
|59 | 8 | 0 | -2.675136 | 0.703195 | 0.206742 |
|60 | 6 | 0 | -4.063093 | 2.599369 | 0.155498 |
|61 | 6 | 0 | -4.267383 | 3.968119 | -0.138811 |
|62 | 6 | 0 | -5.156495 | 1.731134 | 0.251692 |
|63 | 6 | 0 | -6.449577 | 2.183967 | 0.078957 |
|64 | 6 | 0 | -6.698154 | 3.526977 | -0.217707 |
|65 | 6 | 0 | -5.603404 | 4.425326 | -0.334121 |
|66 | 6 | 0 | -3.199070 | 4.925079 | -0.282862 |
|67 | 6 | 0 | -5.858818 | 5.796635 | -0.646512 |
|68 | 6 | 0 | -4.783521 | 6.710930 | -0.774390 |
|69 | 6 | 0 | -3.449125 | 6.220462 | -0.584946 |
|70 | 6 | 0 | -8.036046 | 4.016869 | -0.407634 |
|71 | 6 | 0 | -8.271047 | 5.315822 | -0.700552 |
|72 | 6 | 0 | -7.190535 | 6.254158 | -0.832591 |
|73 | 6 | 0 | -7.415694 | 7.599534 | -1.137670 |
|74 | 6 | 0 | -6.354532 | 8.488063 | -1.260888 |
|75 | 6 | 0 | -5.049539 | 8.048969 | -1.081234 |
|76 | 1 | 0 | -4.980941 | 0.688272 | 0.484485 |
|77 | 1 | 0 | -7.284611 | 1.497075 | 0.177322 |
|78 | 1 | 0 | -2.183403 | 4.588552 | -0.137210 |
|79 | 1 | 0 | -2.625106 | 6.920417 | -0.690130 |
|80 | 1 | 0 | -8.857368 | 3.313484 | -0.310578 |
|81 | 1 | 0 | -9.286105 | 5.674698 | -0.842962 |
|82 | 1 | 0 | -8.435365 | 7.945638 | -1.278500 |
|83 | 1 | 0 | -6.546878 | 9.529252 | -1.498448 |
|84 | 1 | 0 | -4.220795 | 8.744121 | -1.178083 |
|85 | 6 | 0 | -2.710084 | 2.043990 | 0.400180 |
|86 | 8 | 0 | -1.723420 | 2.660760 | 0.749413 |
|87 | 8 | 0 | -2.444536 | -2.025174 | -0.148070 |
|88 | 6 | 0 | -2.275436 | -3.342972 | -0.376080 |
|89 | 8 | 0 | -1.223882 | -3.790046 | -0.788778 |
|90 | 6 | 0 | -3.452324 | -4.184093 | -0.034580 |
|91 | 6 | 0 | -4.799556 | -3.752157 | 0.001307 |
|92 | 6 | 0 | -3.131998 | -5.512197 | 0.263299 |
|93 | 6 | 0 | -5.797875 | -4.699572 | 0.380089 |
|94 | 6 | 0 | -5.240985 | -2.428267 | -0.365705 |
|95 | 6 | 0 | -4.099435 | -6.421323 | 0.639615 |
|96 | 1 | 0 | -2.092889 | -5.813306 | 0.204289 |
|97 | 6 | 0 | -7.176096 | -4.319493 | 0.429376 |
|98 | 6 | 0 | -5.440193 | -6.034795 | 0.711915 |
|99 | 6 | 0 | -6.548410 | -2.080867 | -0.328603 |
|100| 1 | 0 | -4.507985 | -1.700412 | -0.678463 |
|101| 1 | 0 | -3.823816 | -7.442538 | 0.883174 |
|102| 6 | 0 | -7.567223 | -3.002826 | 0.080279 |
|103| 6 | 0 | -8.167115 | -5.257930 | 0.823683 |
|104| 6 | 0 | -6.463259 | -6.963906 | 1.107563 |
|    |    |   |     |     |     |
|----|----|---|-----|-----|-----|
|105 | 1  | 0 | -6.848750 | -1.079017 | -0.622789 |
|106 | 6  | 0 | -8.917926 | -2.645495 |  0.133250 |
|107 | 6  | 0 | -9.506930 | -4.862043 |  0.867757 |
|108 | 6  | 0 | -7.762108 | -6.594021 |  1.164041 |
|109 | 1  | 0 | -6.163701 | -7.976365 |  1.360203 |
|110 | 6  | 0 | -9.878608 | -3.567615 |  0.526118 |
|111 | 1  | 0 | -9.208799 | -1.634878 | -0.138219 |
|112 | 1  | 0 | -10.260000 | -5.582754 |  1.172371 |
|113 | 1  | 0 | -8.526658 | -7.304282 |  1.464551 |
|114 | 1  | 0 | -10.923553 | -3.277625 |  0.564277 |
|115 | 47 | 0 | 6.095167  | -0.072893 |  0.048353 |

SCF Done:  E(RCAM-B3LYP) = -3210.52584544
Full mass-weighted force constant matrix:
Low frequencies --- -3.6396  -0.0016  -0.0009  0.0012  3.2282
3.9189
Low frequencies ---  8.4815   9.4420  10.6553
\( p-(P,S)-3: \text{Ag} \) conformer b

**Standard orientation:**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 1.722014    | 1.472635    | 1.731772    |
| 2             | 6             | 0           | 2.909155    | 1.871087    | 1.130398    |
| 3             | 6             | 0           | 1.771115    | 0.611004    | 2.829191    |
| 4             | 6             | 0           | 3.002915    | 0.173097    | 3.328397    |
| 5             | 6             | 0           | 4.176886    | 0.575122    | 2.727751    |
| 6             | 6             | 0           | 4.145688    | 1.425842    | 1.610275    |
| 7             | 1             | 0           | 0.778371    | 1.818198    | 1.324656    |
| 8             | 1             | 0           | 2.874532    | 2.529100    | 0.268883    |
| 9             | 1             | 0           | 3.010702    | -0.485661   | 4.189324    |
| 10            | 1             | 0           | 5.129860    | 0.232387    | 3.116370    |
| 11            | 6             | 0           | 5.363956    | 1.822950    | 0.968461    |
| 12            | 6             | 0           | 6.398801    | 2.191875    | 0.427660    |
| 13            | 6             | 0           | 7.527959    | 2.940300    | -0.061496   |
| 14            | 6             | 0           | 7.530240    | 4.327127    | 0.123010    |
| 15            | 6             | 0           | 8.624226    | 2.329704    | -0.712186   |
| 16            | 6             | 0           | 8.592146    | 5.099640    | -0.323208   |
| 17            | 6             | 0           | 9.673874    | 4.497422    | -0.959882   |
| 18            | 6             | 0           | 9.689937    | 3.124590    | -1.152000   |
| 19            | 6             | 0           | 8.692388    | 0.917552    | -0.943155   |
| 20            | 6             | 0           | 8.849539    | -0.266142   | -1.187577   |
| 21            | 6             | 0           | 9.155237    | -1.631596   | -1.494521   |
| 22            | 6             | 0           | 10.434140   | -1.933916   | -1.977719   |
| 23            | 6             | 0           | 10.785171   | -3.241451   | -2.276986   |
| 24            | 6             | 0           | 9.863224    | -4.269392   | -2.099725   |
| 25            | 6             | 0           | 8.590062    | -3.987290   | -1.627055   |
| 26            | 6             | 0           | 8.217211    | -2.674697   | -1.319737   |
| 27            | 6             | 0           | 6.879008    | -2.435011   | -0.848306   |
| 28            | 6             | 0           | 5.698404    | -2.487677   | -0.531742   |
| 29            | 6             | 0           | 4.303682    | -2.517754   | -0.203162   |
| 30            | 6             | 0           | 3.376234    | -1.913529   | -1.070077   |
| 31            | 6             | 0           | 3.848187    | -3.091414   | 0.987677    |
| 32            | 6             | 0           | 2.043377    | -1.849669   | -0.727932   |
| 33            | 6             | 0           | 1.604900    | -2.382525   | 0.490531    |
| 34            | 6             | 0           | 2.504540    | -3.034481   | 1.335104    |
| 35            | 8             | 0           | 0.685847    | 0.123651    | 3.484528    |
| 36            | 8             | 0           | 0.291683    | -2.205096   | 0.752999    |
| 37            | 1             | 0           | 6.687045    | 4.790775    | 0.622119    |
| 38            | 1             | 0           | 8.575228    | 6.173316    | -0.171583   |
| 39            | 1             | 0           | 10.506589   | 5.098180    | -1.308780   |
| 40            | 1             | 0           | 10.528937   | 2.650575    | -1.648515   |
| 41            | 1             | 0           | 11.149102   | -1.130225   | -2.111633   |
| 42            | 1             | 0           | 11.780919   | -3.458353   | -2.647842   |
| 43            | 1             | 0           | 10.134556   | -5.293477   | -2.331613   |
| 44            | 1             | 0           | 7.866877    | -4.783300   | -1.491194   |
| 45            | 1             | 0           | 3.718825    | -1.478642   | -2.002989   |
| 46            | 1             | 0           | 4.553254    | -3.575227   | 1.654902    |
| 47            | 1             | 0           | 1.319151    | -1.367523   | -1.374614   |
| 48            | 1             | 0           | 2.173924    | -3.486074   | 2.262295    |
| 49            | 6             | 0           | -0.228048   | -2.441425   | 2.056339    |
|   |   |   | x   | y   | z   |
|---|---|---|-----|-----|-----|
|50 | 6 | 0 | -0.617333 | 0.590264 | 3.167259 |
|51 | 1 | 0 | 0.484503  | -2.132769 | 2.823976 |
|52 | 1 | 0 | -0.461975 | -3.503388 | 2.180483 |
|53 | 1 | 0 | -1.219063 | 0.399279  | 4.058141 |
|54 | 1 | 0 | -0.606713 | 1.667308  | 2.983764 |
|55 | 6 | 0 | -1.498822 | -1.619207 | 2.184679 |
|56 | 6 | 0 | -1.251186 | -0.119285 | 1.965505 |
|57 | 1 | 0 | -1.952263 | -1.791872 | 3.162924 |
|58 | 1 | 0 | -0.651934 | 0.019362  | 1.066011 |
|59 | 8 | 0 | -2.530009 | 0.488093  | 1.765086 |
|60 | 6 | 0 | -3.957116 | 2.047421  | 0.729259 |
|61 | 6 | 0 | -4.244532 | 3.231049  | 0.003069 |
|62 | 6 | 0 | -5.005917 | 1.256730  | 1.216225 |
|63 | 6 | 0 | -6.325910 | 1.591242  | 0.993168 |
|64 | 6 | 0 | -6.654528 | 2.743464  | 0.274729 |
|65 | 6 | 0 | -5.611800 | 3.572647  | -0.219840|
|66 | 6 | 0 | -3.238726 | 4.120941  | -0.521912|
|67 | 6 | 0 | -5.954209 | 4.754350  | -0.948903|
|68 | 6 | 0 | -4.936707 | 5.602614  | -1.451601|
|69 | 6 | 0 | -3.571919 | 5.240392  | -1.206448|
|70 | 6 | 0 | -8.023694 | 3.104368  | 0.028409 |
|71 | 6 | 0 | -8.339658 | 4.221966  | -0.663633|
|72 | 6 | 0 | -7.315759 | 5.089316  | -1.177416|
|73 | 6 | 0 | -7.625428 | 6.248772  | -1.893940|
|74 | 6 | 0 | -6.619562 | 7.073936  | -2.382158|
|75 | 6 | 0 | -5.286379 | 6.754683  | -2.163277|
|76 | 1 | 0 | -4.773910 | 0.361920  | 1.778166 |
|77 | 1 | 0 | -7.117123 | 0.950597  | 1.369925 |
|78 | 1 | 0 | -2.201296 | 3.873957  | -0.358832|
|79 | 1 | 0 | -2.791402 | 5.892672  | -1.588023|
|80 | 1 | 0 | -8.801188 | 2.452470  | 0.414675 |
|81 | 1 | 0 | -9.377644 | 4.485402  | -0.844207|
|82 | 1 | 0 | -8.667886 | 6.499605  | -2.066585|
|83 | 1 | 0 | -6.877623 | 7.970393  | -2.936516|
|84 | 1 | 0 | -4.499846 | 7.398989  | -2.545056|
|85 | 6 | 0 | -2.567989 | 1.589300  | 0.978900 |
|86 | 8 | 0 | -1.544571 | 2.091012  | 0.553238 |
|87 | 8 | 0 | -2.391054 | -2.085408 | 1.171143 |
|88 | 6 | 0 | -3.692176 | -2.257934 | 1.498562 |
|89 | 8 | 0 | -4.102670 | -2.048999 | 2.622490 |
|90 | 6 | 0 | -4.489715 | -2.723583 | 0.334223 |
|91 | 6 | 0 | -5.905321 | -2.784118 | 0.363918 |
|92 | 6 | 0 | -3.799446 | -3.115391 | -0.819151|
|93 | 6 | 0 | -6.587827 | -3.244339 | -0.801295|
|94 | 6 | 0 | -6.706307 | -2.391764 | 1.497684 |
|95 | 6 | 0 | -4.465138 | -3.571510 | -1.938788|
|96 | 1 | 0 | -2.718897 | -3.060798 | -0.824461|
|97 | 6 | 0 | -8.016115 | -3.311302 | -0.825877|
|98 | 6 | 0 | -5.860247 | -3.643768 | -1.954631|
|99 | 6 | 0 | -8.058615 | -2.453159 | 1.463906 |
|100| 1 | 0 | -6.201079 | -2.055494 | 2.389946 |
|101| 1 | 0 | -3.905463 | -3.875683 | -2.817697|
|102| 6 | 0 | -8.768868 | -2.914603 | 0.307294 |
|103| 6 | 0 | -8.694298 | -3.774627 | -1.984972|
|104| 6 | 0 | -6.570804 | -4.111007 | -3.113382|
SCF Done:  E(RCAM-B3LYP) = -3210.52574322   A.U. after 19 cycles
Full mass-weighted force constant matrix:
  Low frequencies ---  -0.0015  -0.0010  0.0004   2.6483   4.1784
  4.9277
  Low frequencies ---   8.8626   9.4473  12.4471
### Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -2.286915   | 2.171959   | 2.414612    |
| 2             | 6             | 0           | -3.635938   | 2.241290   | 2.090453    |
| 3             | 6             | 0           | -1.357402   | 1.880908   | 1.416046    |
| 4             | 6             | 0           | -1.771796   | 1.736980   | 0.086408    |
| 5             | 6             | 0           | -3.109778   | 1.814495   | -0.230783   |
| 6             | 6             | 0           | -4.065951   | 2.041782   | 0.775509    |
| 7             | 1             | 0           | -1.975722   | 2.327063   | 3.440158    |
| 8             | 1             | 0           | -4.363973   | 2.436546   | 2.870292    |
| 9             | 1             | 0           | -1.024064   | 1.951308   | 0.117000    |
| 10            | 1             | 0           | -3.433884   | 1.677455   | -1.257093   |
| 11            | 6             | 0           | -5.460070   | 2.003411   | 0.444004    |
| 12            | 6             | 0           | -6.636087   | 1.951308   | 0.117000    |
| 13            | 6             | 0           | -8.002381   | 2.197345   | -0.625524   |
| 14            | 6             | 0           | -8.526526   | 3.479683   | -0.071348   |
| 15            | 6             | 0           | -8.821479   | 1.196515   | -0.837034   |
| 16            | 6             | 0           | -9.832031   | 3.774070   | -0.434913   |
| 17            | 6             | 0           | -10.636372  | 2.790326   | -1.003480   |
| 18            | 6             | 0           | -10.135382  | 1.513057   | -1.203098   |
| 19            | 6             | 0           | -8.361136   | -0.142794  | -1.053146   |
| 20            | 6             | 0           | -8.074669   | -1.305826  | -1.264380   |
| 21            | 6             | 0           | -7.847226   | -2.687407  | -1.580035   |
| 22            | 6             | 0           | -8.825067   | -3.366929  | -2.317059   |
| 23            | 6             | 0           | -8.655127   | -4.700494  | -2.657237   |
| 24            | 6             | 0           | -7.504087   | -5.378070  | -2.265350   |
| 25            | 6             | 0           | -6.527447   | -4.722281  | -1.530898   |
| 26            | 6             | 0           | -6.680789   | -3.377240  | -1.173358   |
| 27            | 6             | 0           | -5.635646   | -2.756044  | -0.405978   |
| 28            | 6             | 0           | -4.648735   | -2.513679  | 0.277103    |
| 29            | 6             | 0           | -3.492453   | -2.256656  | 1.084063    |
| 30            | 6             | 0           | -2.203048   | -2.438975  | 0.572058    |
| 31            | 6             | 0           | -3.640858   | -1.795347  | 2.403462    |
| 32            | 6             | 0           | -1.080039   | -2.148633  | 1.337963    |
| 33            | 6             | 0           | -1.248273   | -1.658589  | 2.634133    |
| 34            | 6             | 0           | -2.532369   | -1.499013  | 3.166552    |
| 35            | 8             | 0           | -0.333375   | 1.706828   | 1.621629    |
| 36            | 8             | 0           | -0.240983   | -1.288554  | 3.466643    |
| 37            | 1             | 0           | -7.894015   | 4.243146   | 0.367315    |
| 38            | 1             | 0           | -10.220737  | 4.773937   | -0.276019   |
| 39            | 1             | 0           | -11.657231  | 3.017253   | -1.290618   |
| 40            | 1             | 0           | -10.758454  | 0.742544   | -1.642653   |
| 41            | 1             | 0           | -9.718284   | -2.833474  | -2.621450   |
| 42            | 1             | 0           | -9.421854   | -5.209896  | -3.230162   |
| 43            | 1             | 0           | -7.366572   | -6.420811  | -2.529730   |
| 44            | 1             | 0           | -5.631167   | -5.246572  | -1.219741   |
| 45            | 1             | 0           | -2.075538   | -2.798805  | -0.442728   |
| 46            | 1             | 0           | -4.635216   | -1.661461  | 2.816403    |
| 47            | 1             | 0           | -0.093633   | -2.283925  | 0.908374    |
| 48            | 1             | 0           | -2.632300   | -1.132806  | 4.182017    |
| 49            | 6             | 0           | 1.114186    | -1.537728  | 3.126407    |
|   |     |     |         |         |         |
|---|-----|-----|---------|---------|---------|
|50 | 6   | 0   | 0.497793| 1.617874| 2.938342|
|51 | 1   | 0   | 1.217809| -2.518671| 2.656123|
|52 | 1   | 0   | 1.652955| -1.553027| 4.076092|
|53 | 1   | 0   | 0.635685| 2.619879 | 3.356606|
|54 | 1   | 0   | -0.160771| 1.037844 | 3.587626|
|55 | 6   | 0   | 1.740903| -0.480592| 2.208813|
|56 | 6   | 0   | 1.841635| 0.921433 | 2.817963|
|57 | 1   | 0   | 1.216779| -0.422981| 1.254953|
|58 | 1   | 0   | 2.332798| 0.880767 | 3.793367|
|59 | 8   | 0   | 2.633773| 1.720008 | 1.930983|
|60 | 6   | 0   | 4.633494| 2.852190 | 1.287231|
|61 | 6   | 0   | 4.088394| 3.535154 | 0.170499|
|62 | 6   | 0   | 6.009699| 2.917585 | 1.539471|
|63 | 6   | 0   | 6.869405| 3.614132 | 0.716897|
|64 | 6   | 0   | 6.378597| 4.292296 | -0.409212|
|65 | 6   | 0   | 4.984145| 4.260966 | -0.675613|
|66 | 6   | 0   | 2.684630| 3.572003 | -0.166617|
|67 | 6   | 0   | 4.493081| 4.971724 | -1.816864|
|68 | 6   | 0   | 3.108395| 4.972907 | -2.116717|
|69 | 6   | 0   | 2.229972| 4.251325 | -1.245237|
|70 | 6   | 0   | 7.259610| 5.021675 | -1.271497|
|71 | 6   | 0   | 6.787968| 5.685155 | -2.350180|
|72 | 6   | 0   | 5.385589| 5.685263 | -2.661852|
|73 | 6   | 0   | 4.881557| 6.369258 | -3.771378|
|74 | 6   | 0   | 3.521596| 6.361785 | -4.056045|
|75 | 6   | 0   | 2.641336| 5.670386 | -3.235121|
|76 | 1   | 0   | 6.389994| 2.395654 | 2.408861|
|77 | 1   | 0   | 7.932869| 3.638846 | 0.932928|
|78 | 1   | 0   | 1.980751| 3.040804 | 0.453854|
|79 | 1   | 0   | 1.166425| 4.257693 | -1.467315|
|80 | 1   | 0   | 8.319755| 5.025633 | -1.037327|
|81 | 1   | 0   | 7.462055| 6.233422 | -3.001650|
|82 | 1   | 0   | 5.569702| 6.910921 | -4.413956|
|83 | 1   | 0   | 3.147285| 6.898633 | -4.921656|
|84 | 1   | 0   | 1.577731| 5.664921 | -3.454862|
|85 | 6   | 0   | 3.892741| 2.032330 | 2.287881|
|86 | 8   | 0   | 4.383767| 1.651614 | 3.331750|
|87 | 8   | 0   | 3.086156| -0.908358 | 1.979048|
|88 | 6   | 0   | 3.294460| -1.772273 | 0.958740|
|89 | 8   | 0   | 2.365115| -2.215096 | 0.310656|
|90 | 6   | 0   | 4.736668| -2.069854 | 0.775258|
|91 | 6   | 0   | 5.193135| -3.079720 | -0.108691|
|92 | 6   | 0   | 5.660665| -1.312975 | 1.507700|
|93 | 6   | 0   | 6.599135| -3.290907 | -0.226384|
|94 | 6   | 0   | 4.322006| -3.922112 | -0.890070|
|95 | 6   | 0   | 7.019607| -1.517873 | 1.381632|
|96 | 1   | 0   | 5.299523| -0.550272 | 2.185311|
|97 | 6   | 0   | 7.109640| -4.303274 | -1.097734|
|98 | 6   | 0   | 7.513852| -2.500617 | 0.520357|
|99 | 6   | 0   | 4.813669| -4.881049 | -1.709435|
|100| 1   | 0   | 3.256678| -3.770309 | -0.811057|
|101| 1   | 0   | 7.714848| -0.912860 | 1.955125|
|102| 6   | 0   | 6.221409| -5.111410 | -1.849792|
|103| 6   | 0   | 8.510027| -4.510570 | -1.216479|
|104| 6   | 0   | 8.925880| -2.728458 | 0.379378|
|   |   |   | 4.132277 | -5.501948 | -2.284244 |
|---|---|---|----------|-----------|-----------|
| 105 | 1 | 0 | 6.734957 | -6.099672 | -2.695661 |
| 106 | 6 | 0 | 8.984916 | -5.507782 | -2.073017 |
| 107 | 6 | 0 | 9.401409 | -3.685905 | -0.448257 |
| 108 | 1 | 0 | 9.603811 | -2.109448 | 0.959017 |
| 109 | 6 | 0 | 8.105005 | -6.295306 | -2.805490 |
| 110 | 1 | 0 | 6.047015 | -6.715062 | -3.267956 |
| 111 | 6 | 0 | 10.056345 | -5.662158 | -2.160231 |
| 112 | 1 | 0 | 10.470394 | -3.850365 | -0.546610 |
| 113 | 1 | 0 | 8.490684 | -7.065620 | -3.465322 |
| 114 | 47 | 0 | -5.998116 | -0.398095 | -0.059096 |

**SCF Done:** $E_{(RCAM-B3LYP)} = -3210.52391368$

**Full mass-weighted force constant matrix:**

| Low frequencies | -0.0017 | 0.0003 | 0.0008 | 1.0985 | 3.8260 |
|-----------------|---------|--------|--------|--------|-------|
| 4.7578          |         |        |        |        |       |

| Low frequencies | 7.5264 | 10.6455 | 12.2064 |
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