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Keywords:	Vibrational Circular Dichroism (VCD), ruthenium complex, planar chirality, chiral metal complex, anharmonicity

Mid-IR and CH stretching VCD spectroscopy to distinguish various sources of chirality: The case of quinophaneoxazoline based ruthenium(II) complexes

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Abstract

Five diastereomers of ruthenium(II) complexes based on quinolinophaneoxazoline ligands were investigated by vibrational circular dichroism (VCD) in the mid-IR and

CH stretching regions. Diastereomers differ in three sources of chirality: the planar chirality of the quinolinophane moiety, the central chirality of an asymmetric carbon atom of the oxazoline ring, and the chirality of the ruthenium atom. VCD, allied to DFT calculations, has been found to be effective in disentangling the various forms of chirality. In particular, a VCD band is identified in the CH stretching region directly connected to the chirality of the metal. The analysis of the calculated VCD spectra is carried out by partitioning the complexes into fragments. The anharmonic analysis is also performed with a recently proposed reduced-dimensionality approach: such treatment is particularly important when examining spectroscopic regions highly perturbed by resonances,like the CH stretching region.

Keywords

Vibrational circular dichroism (VCD); ruthenium complex; planar chirality; chiral metal complex; anharmonicity

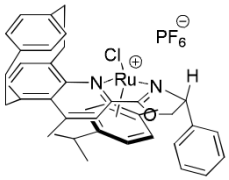
Introduction

Vibrational circular dichroism (VCD) spectroscopy has emerged as one of the most reliable spectroscopic techniques for investigating the absolute configuration of chiral molecules.[1–3] In particular, in combination with Density Functional Theory (DFT) calculations,[4] VCD has made it possible to determine the relative configuration of chiral molecules possessing multiple chiral centers, such as in natural products, or to monitor various forms of configuration, planar, axial, central, etc.[5–13] If compared with the parent technique of UV-visible circular dichroism, i.e. electronic circular dichroism (ECD), while this latter is superior for use of smaller sample quantities, VCD, like most forms of vibrational spectroscopies, is more adequate to discriminate various sources of chirality within molecular systems. Moreover due to its higher sensitivity, VCD can help to investigate conformational aspects as well, whose

contributions are often hidden in ECD spectra. VCD spectroscopy has been increasingly appreciated outside the fields in which the technique was initially developed, namely the spectroscopic chemical-physical field. Indeed, for some years now, the number of researcher who use this tool, including organic chemists, natural products experts, drug design scientists and materials science experts, has been growing significantly. This expansion was facilitated by the advent of easy-to-use commercial instruments and user-friendly DFT packages. In most problems one can be satisfied with the standard approach proposed by DFT programs within the harmonic-oscillator approximation and with a qualitative comparison between experimental and calculated spectra.[4,14–16] Nonetheless, "harmonic" simulations require *ad-hoc* scaling factors of the wavenumber to be compared to experimental data, and fail when anhamonic effects play crucial roles as in the case of resonances that strongly perturb the normal mode descriptions. Yet, recently some progress has been made beyond the harmonic approximation,[17–21] a step that may need to be addressed even in "complicated cases", or in treating large sets of conformations with unbiased comparisons of experiments and calculations.[22,23] Anharmonic treatment allows one to avoid *ad-hoc* scaling factors, and unlocks to the interpretation regions of the spectra otherwise forbidden.

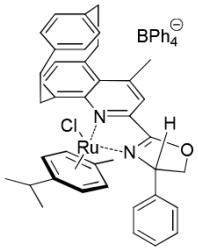
Among the many compounds investigated by VCD, there are many examples of transition metal complexes.[24–32] The profound connection between chirality and metal complexes has been highlighted since the dawn of coordination chemistry. In fact, chiral metal complexes were isolated only a few years after the foundation of coordination chemistry[33] and since then chiral organometallic complexes have been used in various fields, as homogeneous catalysts, as organic light-emitting devices (OLEDs), as well as in devices for biological imaging.[34–39] Depending on the metal and its oxidation states, different coordination numbers and geometries are allowed, therefore, when the metal is surrounded by ligands, different sources within the complex can contribute to molecular chirality overall.[40] This makes the study of strereochemistry in transition metal complexes a challenging and active field, where the combination of more than one chiroptical spectroscopy is often necessary to obtain a complete

understanding of the system under investigation.[41–43] In this context, VCD spectroscopy has played a crucial role by allowing us to recognize the various contributions deriving from different portions of the complexes and/or due to the conformational flexibility of the systems.[29,44–46]



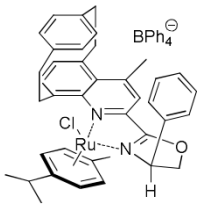
-470

1a: S_p, R, S_M-**1**$^+$ PF_6^-



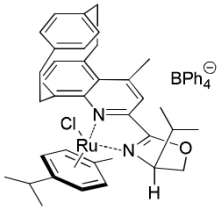
+422

1b:R_p, S, R_M-**1**$^+$ BPh_4^-



+298

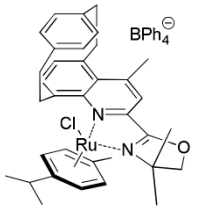
1c: R_p, R, R_M-**1**$^+$ BPh_4^-



1: [RuCl(η^6-p-cym)(QUINEPHOX)]$^+$

2: [RuCl(η^6-p-cym)(QUINEPROX)]$^+$

3: [RuCl(η^6-p-cym)(QUINEDIMOX)]$^+$



+221

2c: R_p, R, R_M-**2**$^+$ BPh_4^-

+357

3c: R_p, R_M-**3**$^+$ BPh_4^-

Scheme 1: Studied ruthenium complexes prepared from the dimer (η^6-p-cymene)ruthenium(II) and the corresponding quinolinophaneoxaline-based ligands.[47] (Experimental values of the specific optical rotation measured at 589 nm, RT, in $CHCl_3$ solutions are given).

Here, we deal with one of these "complicated case", in which three elements contribute to the chirality in each of the five quinolinophaneoxazoline (η^6-p-cymene)ruthenium(II) complexes (Scheme 1), i.e. planar chirality, central chirality (due to the presence of a stereogenic carbon) and chirality of the metal center (ruthenium).[47] Previous investigations on free paraquinolinophane ligands have allowed us to disentangle the planar and central chirality by VCD,[48] or, in other Ruthenium (II) complexes, to disentangle the central chirality from the metal chirality.[32] The use of sensitive spectroscopy is essential since epimerization can occur in solution, so under such conditions it is important to assign the configuration to

the metal. To our knowledge, no study has been attempted, so far, with the three forms of chirality present simultaneously together, although a previous investigation, based on X-ray diffraction experiments, helped to define the configuration of the complexes, with the ECD used as an auxiliary tool in a limited spectroscopic region.[47] Here, we wish to define whether, usign different and independent regions of the VCD/IR spectra, it is possible to obtain responses, individually associated with the three types of chirality.

Experimental Methods

All VCD measurements were performed on CCl_4 solutions with a Jasco FVS6000 VCD apparatus. In the mid-IR region BaF_2 cells with a path length of 200 μm were used, while, for the CH stretching region, 1 mm quartz infrasil cuvettes were used. In the first case, a liquid N_2-cooled MCT detector was mounted on the instrument,while in the second case a liquid N_2-cooled InSb detector was used. In both cases the concentration of the solutions was approx. 0.2 M. For each sample, 6000 scans were carried out. The spectra of the solvent were taken under the same conditions. The latter were subtracted from the spectra in solution for both IR absorption and VCD.

Computational Details

Unless otherwise specified, calculations were performed with the GAUSSIAN16 suite of quantum chemistry programs.[49] The combination of the B3PW91[50] functional and SNSD basis set on light atoms[51] and of the LanL2DZ basis set with effective core potentials to replace core electrons on ruthenium atom was employed.[52] Empirical dispersions (D3BJ) were also included. This combination will be referred to in the text as PW91.

The initial geometries for each complex were taken from ref. 47, then conformational searches were performed with the CREST code[53] with the semiempirical extended tight-binding (TB) quantum chemistry method, GFN2-xTB.[54] The most stable conformers were

re-optimized at the DFT level. Geometry optimizations were performed with tight convergence criteria (i.e. 1×10^{-5} hartree/bohr and 4×10^{-5} bohr on RMS forces and displacements, respectively, with thresholds for the maximum values being 1.5 times larger) and the minima were confirmed by Hessian evaluations. The harmonic energies and intensities were obtained using the analytical second derivatives of the energy and first derivatives of the properties of interest. Higher-order derivatives, needed for anharmonic calculations were computed through numerical differentiations using 0.01 $\sqrt{\text{amu}}$ Å for the displacements along the mass-weighted normal coordinates.

Anharmonic calculations were performed using a reduced-dimensionality (RD) scheme within the second-order vibrational perturbation theory (VPT2).[55,56] Derivatives were computed along all the CH-stretching normal modes defining the initial subset of normal modes. The normal modes coupled to the selected ones were identified with a threshold of $\bar{\alpha}_i(j) = 0.015$, ensuring that all modes interacting by Darling—Dennison resonances were included,[56] $\bar{\alpha}_i(j)$ corresponds to the absolute values of

$$\alpha_i(j) = \frac{\mathsf{f}_{iij}}{4\omega_j}$$

This quantity can be used as gauge to evaluate the impact of excluded j-normal mode on the anharmonic correction to the energy.

The subset was then completed including 2-quanta transitions falling within the spectroscopic range of interest, a condition that was checked by evaluating their harmonic frequencies after applying a 0.94 scaling factor.

Anharmonic calculations were performed with a development version of the Gaussian suite of programs.[57] Diverging terms are removed from the perturbative expressions (therefore leading to the so-called IDVPT2[58] level), and then reintroduced through a variational step in the GVPT2 framework.[59]

To match experimental conditions (CCl_4 solutions), the solvent effects were simulated

using the polarizable continuum model (PCM) in its integral equation formalism,[60] with the default parameters of GAUSSIAN16.[49]

Results and Discussions

OR and ECD spectra

We begin our analysis by briefly examining chiroptical data other than VCD data, namely the specific optical rotation (OR) data at 589 nm and ambient temperature, and the electronic circular dichroism (ECD) spectra. While the former have been in part re-measured here and are reported in Scheme 1; the latter, with the exception of compounds **1a** and **1b**, were not re-measured so they are not reported and can be found in ref. 47. The new ECD spectra are given in Supplementary Material in Figure S1. The absolute values of OR range from 221 to 470, which can be considered fairly large even though they are typical of some cyclophane systems.[61–63] From a raw estimatite, it appears that the positive OR is associated either with the paracycloquinolinophane R_P or with the R_M metal configuration, or the simultaneous presence of both, while the central configuration of the carbon atom of the oxazoline ring does not seem to be relevant: the negative OR value appears associated with the paracycloquinolinophane configuration S_P or with the metal configuration S_M. Since the positive OR of the "parent" quinolinophanes not complexed with metals[48] was not related to R_P but to the central chirality of an external carbon atom, the positive sign of OR is determined by R_M configuration or by the concurrence of R_P and R_M, which induces a sort of synergistic effect in determining the sign and the magnitude of the OR. The correlation of ECD spectra with R_M is more indirect as per ref. 47, in particularl considering that the Pearson coefficient – which measures the similarity between calculations and experiments – is high only when a limited portion of ECD spectra is considered.

Below, we will show that VCD exhibits many bands and we will look for which ones are associated separately with the planar R_P (S_P), central R (S) and metal R_M (S_M)

configurations, the latter being the most difficult to capture, and yet also our main center of interest.

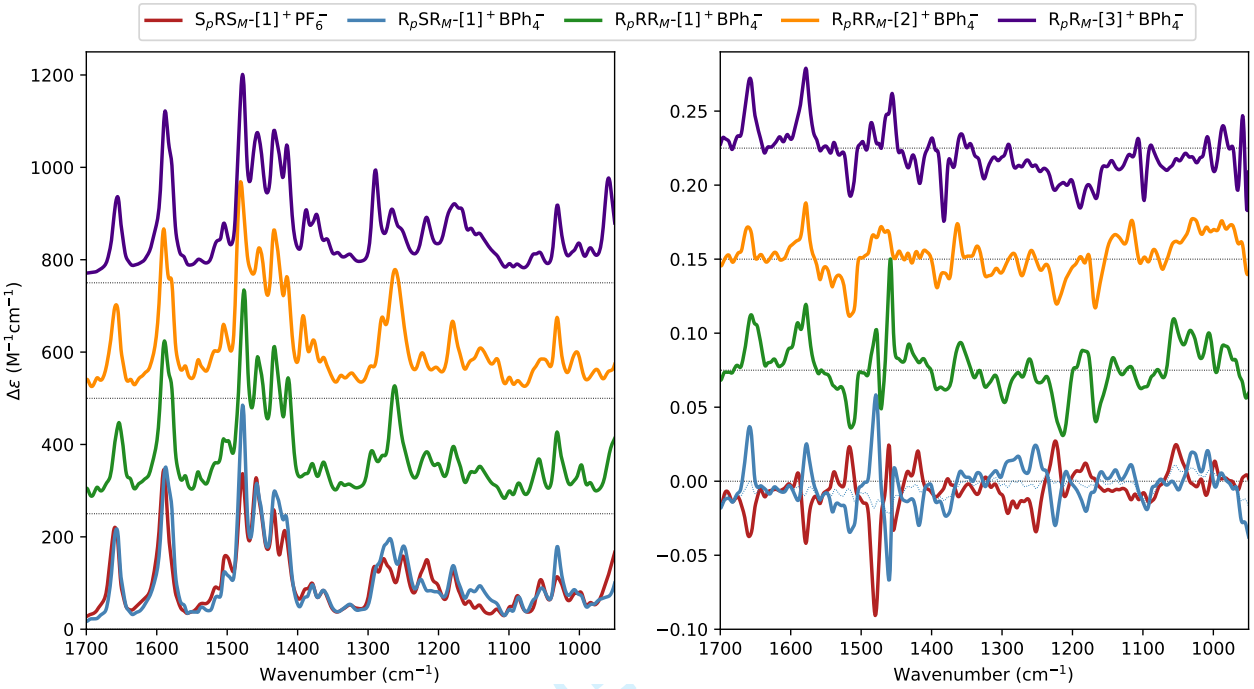


Figure 1: Experimental IR (left) and VCD (right) spectra of all complexes studied in the mid-IR region. CCl_4 solvent with cells of path length of 200 μm and solutions $\approx 4.0 \cdot 10^{-2}$ M. Each color is associated with a different diastereomer recalled in the legend above the figure (see Scheme 1 for the structures).

VCD Spectra: the mid-IR Region

The assignment of the absolute configuration of complexes in Scheme 1 is that proposed in ref. 47, based ultimately on X-ray crystallographic data. In Figure 1, we report the experimental IR and VCD spectra in the mid-IR region. The experimental VCD spectra in Figure 1 contain several bands of opposite sign. First of all, we find it reassuring that the two enantiomers **1a** and **1b** of Scheme 1 have opposite signals for all VCD bands, irrespective of the different counterion. The dominant contributions come from the paracycloquinolinophane moiety. Indeed, the positive (+) VCD band observed in Figure 1 at ca. 1670 cm^{-1} is associated with the R_P configuration, which also determines the (+) band at 1590 cm^{-1}

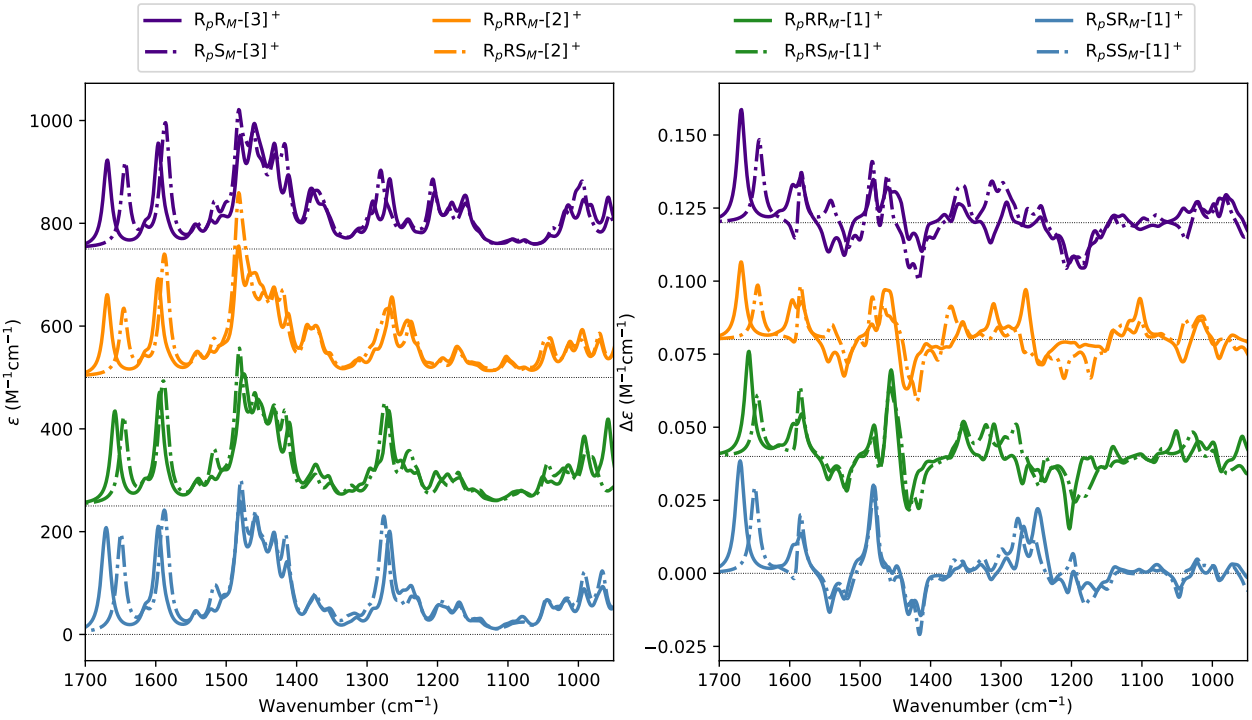


Figure 2: Simulated IR (left) and VCD (right) spectra of all the complexes after conformational weighted average. Results for both configurations in the center of the ruthenium are shown. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 5 cm^{-1} of half-width at half-maximum. A scaling factor of 0.97 was applied to the harmonic frequencies.

and the triplet (−,−,+) at ca. (1550, 1540, 1480 cm^{-1}). The last triplet was observed with the paraquinolinophanes reported in ref. 48, although centered at higher wavenumbers of ca. 30-40 cm^{-1}, and was identified as the signature of the quinolinophane chirality. The behaviour of the complexes identified as **1** in Scheme1, conform better to this observation, while complexes **2** and **3** present some perturbation on the signs of the noted VCD bands. The (+) VCD band at 1460 cm^{-1} also appears related to R_P. The lower-frequency range, below 1300 cm^{-1}, of either the IR and VCD spectra, appears more strongly perturbed by the outer groups of the oxazoline moiety, the differences between the methyl and phenyl substituents being the largest. It is not easy to define from these VCD spectra a signature of the R_M or S_M configuration of the Ru-center. The central R chirality of the ligands is also difficult to associate with specific VCD bands, since the groups bound to the stereocenter are chemically very different.

To get deeper insight, let us now focus on the calculated VCD and IR spectra presented in Figure 2. To facilitate comparison with experiments, a scaling factor of 0.97 was applied to calculated harmonic frequencies. The calculated VCD and IR spectra are in good agreement with the experimental data and they allow us to highlight some important perturbations brought about by the configuration of the metal. In addition to the calculated spectra for the diastereomers actually recorded, in Figure 2 we also report superimposed, the spectra calculated for the diastereomers obtained by inverting the metal configuration. The influence of the latter can be noted in some portions of the spectra. Starting from high wavenumbers, the highest-frequency band in the region, for all four complexes, is expected to be ca. 1680 cm^{-1} for (R_P,R_M), while that for the configuration (R_P,S_M) is approx. 1650 cm^{-1}, without change of sign in both cases. The two VCD components (at about 1550- 1540 cm^{-1}) with the same sign in the characteristic quinolinophane triplet identified in ref. 48 (signature of R_P and R_M for complexes **2** and **3**) are perturbed when switching from R_P to S_P, while no change is noted for all diastereomers of **1**. Finally we observe that in **1c**, **2** and **3** there are notable changes in the signs of the calculated VCD bands at 1260-1310 cm^{-1} on going from R_M to S_M (some changes are also noticed in **1a**). A similar perturbation is noted from R_M to S_M between 1160 and 1190 cm^{-1} for **1a**, **2**, and **3**. Although we consider these results significant, we believe they would be difficult to identify in the experimental data. Comparison of the experimental and calculated signals of 1260–1310 cm^{-1} suggests that the band at 1265 cm^{-1} has a positive and noticeable VCD intensity in the case of R_PSR_M and less intense for R_PSS_M. In contrast, in distareomers **3**, the R diastereomers gives negative contributions to both RR_M and RS_M (see below).

VCD Spectra: the CH Stretching Region

Let us now investigate the CH stretching region (the first two panels on the left of Figure 3 for the experimental data and the last two for the calculated data) where a scaling factor of 0.94 has been applied to the calculated frequencies. Indeed, the CH stretching region was the first

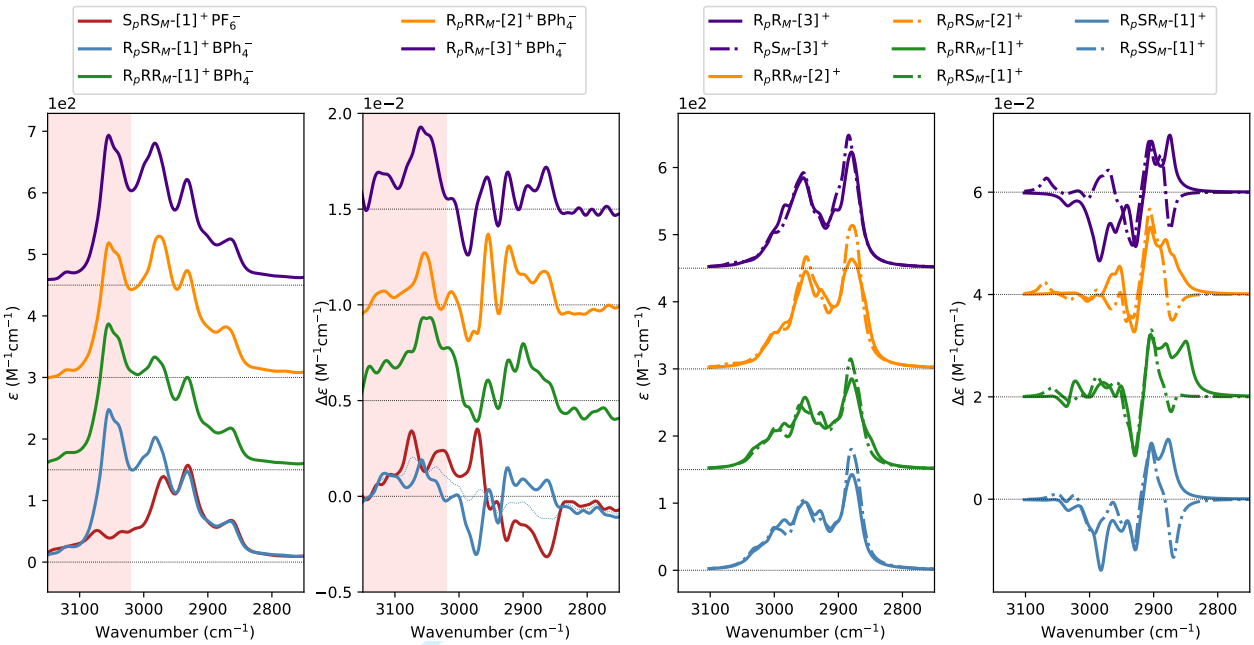


Figure 3: Comparison of the experimental IR and VCD spectra (first two panels) of the ruthenium complexes and the simulated ones (third and fourth panels). The calculations were performed at the PW91 level and both metal center configurations were considered. The spectral band-shape was obtained by applying Lorentzian distribution functions with half width of 10 cm^{-1} at half-maximum. A scaling factor of 0.94 was applied to the harmonic frequencies.

investigated in the 50-year history of the VCD,[64,65] but was subsequently neglected due to computational difficulties. Thanks to recent advances in the treatment anharmonicity,[18,20,21] it is possible to produce more reliable results, which can be compared to experiment with a higher degree of confidence. In fact, in Figure 3, we note that the lowest-frequency portion of the spectrum, around 2860 cm^{-1}, consists in a shoulder of a broader band, and largely the entire region below 2900 cm^{-1} is common to **1b**,**1c**, **2** and **3** (all of R_PR_M type) and of opposite sign for **1a** (R_PR_M). The calculations on the right side of Figure 3, even in the harmonic approximation, predict a (+) VCD feature at approx. 2870 cm^{-1} for (R_PR_M) and a (–) VCD feature there for (R_PS_M). We do not have an experimental counterexample (R_PS_M), but all (R_PR_M)'s appear to have the same trend regardless of the substituents, and for the R_PS_M cases the simulated VCD spectrum is identical except for the first (low energy) VCD band. Therefore, calculations suggest this as a signature of the configuration

at the metal center.

Beyond Visual Inspection and Comparison

To assign the contributions ot the VCD/IR bands of the various moieties of the complexes, we took into consideration the procedure proposed by Hug to define the "quasi-atomic" contribution of each atom to spectroscopic properties.[66,67] The atomic contributions can be combined to generate the contributions of different portions of the molecule to the overall transition, the sum of all contributions gives the overall VCD and IR intensity. Here, we have re-implemented the equations reported in ref. 66 in a prototypical Python code that uses matplotib[68] and Jmol[69] for the 2D and 3D representations.

To investigate the role played by the different sources of chirality in the spectra, we focused our attention on complex **1b** in the most populated conformational state (ca. 99%) and partitioned it into three fragments which were then used to calculate the sub-spectra of each fragment with the method described above. In Figure 4 we have highlighted the quinolinophane portion in green, the metal with added p-cymene coordinated to it in orange and the oxazoline ring attached phenyl group in purple. The sub-spectra of each fragment were simulated by assigning Lorentzian distribution functions with the same value of half-width at half-maximum with respect to the whole spectrum. They are plotted below the simulated spectrum using color maps where negative peaks are shown in red and positive ones in blue. In the right part of the figure some normal modes of interest are shown represented by arrows on atoms whose length is proportional to the atomic displacements. They were selected since they are related to the bands identified as diagnostic in the previous section. The calculated VCD spectra in the CH stretching region for R_PSR_M-**1** (**1b**) and for its diastereomer R_PSS_M-**1** are reported and analysed.

From Figure 4, we can deduce that, even though the three molecular parts interact and provide mixed contributions in several cases, the negative VCD band calculated at 1722 cm^{-1} (re-scaled to 1670 cm^{-1}) and the (-, -, +) triplet of bands between 1617 and 1520 cm^{-1}

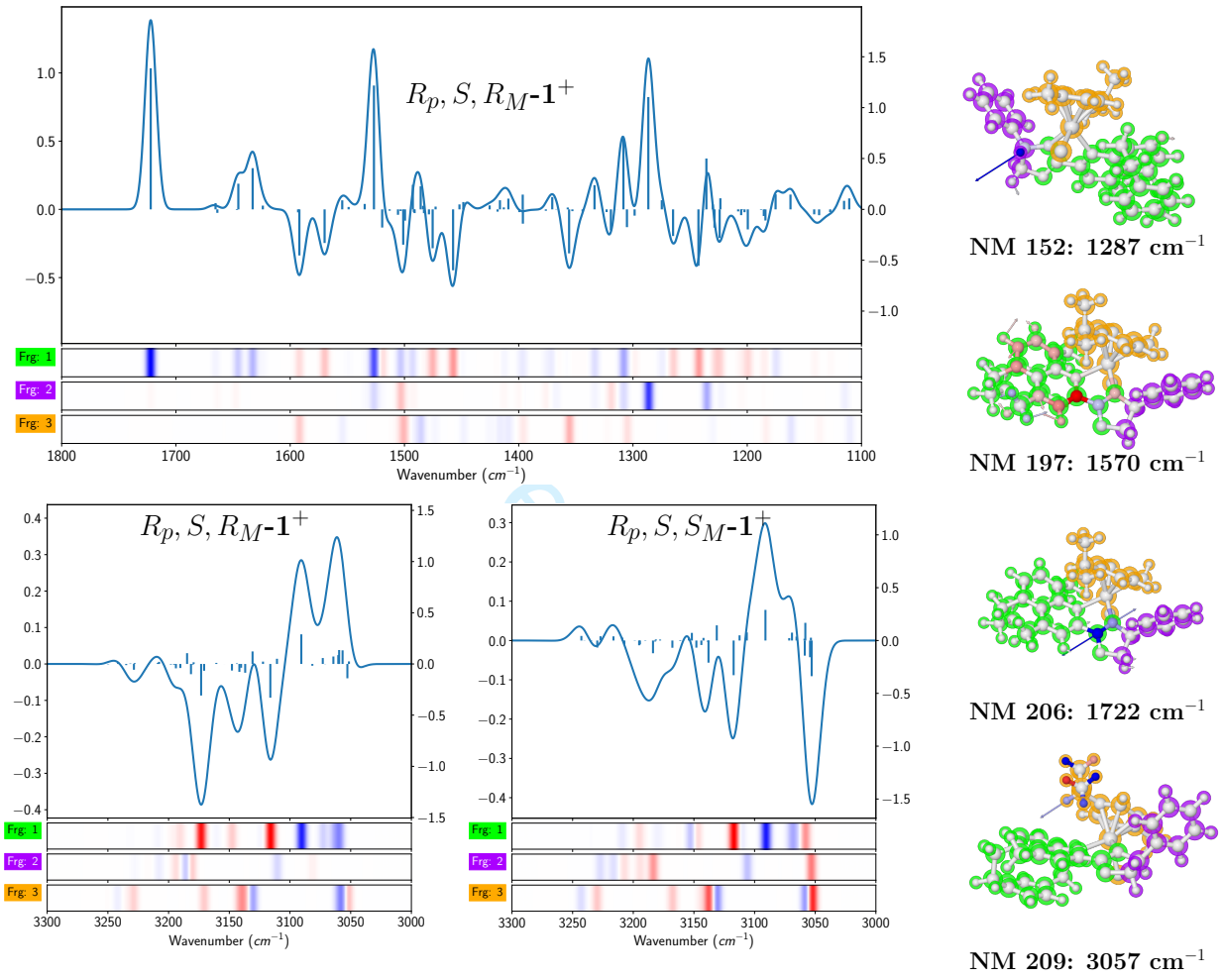


Figure 4: Assignment of the VCD mid-IR and CH stretching bands calculated for the most populated conformer of R_PSR_M-**1** to the normal modes (NMs) located in three fragments (color coded as in the right part of the figure) for four NMs. On the bottom right panel, the assignment of VCD bands for the R_PSS_M-**1** (for which no experimental data is available). The negative (red) and positive (blue) contributions to the VCD bands are reported below the calculated spectra according to which atoms in the 3D model are colored. The contributions were partitioned following the method elaborated in refs. 66,67

are unequivocally attributable to the quinoliphane moiety. Conversely, characteristic band calculated at 1287 cm^{-1} (rescaled at 1250 cm^{-1}) originates from oxazoline ring hosting the external stereocenter, which confirms the correlation suggested above: positive for R_PSS_M and negative for R_PSR_M, independently of the central chirality of the external group. Finally, the characteristic strong VCD band at 2860 cm^{-1}, calculated at 3057 cm^{-1} (positive for **1b** and negative for **1a**) is attributed to the methyl stretchings of the p-cymene moiety and its sign discriminates the configuration of the metal, independently of the planar chirality and therefore directly related to the chirality of the metal.

Anharmonic Calculations Performed with the Reduced Dimensionality Scheme

Since the discrimination between R_M/S_M chirality is focused on a signature in the CH-stretching region, it is important to consider the anharmonicity which has a greater influence in this region of the IR and VCD spectra.[20] However, the size of the systems in terms of the number of atoms considerably impedes the anharmonic calculations of entire molecules even with methodologies rooted in second-order vibrational perturbation theory (VPT2).

With this in mind and with the aim of investigating only the CH stretching region at the anharmonic level, we decided to use a reduced-dimensionality (RD) scheme in our approach.[55,56] In the RD scheme, only a subset of all normal modes, directly related to the regions of interest, are treated at the anharmonic level while the other modes still contribute indirectly to the anharmonicity.[56]

This allows us to sensibly reduce the computational cost. Among the original 246 normal modes, numerical differentiations were performed on less than half of them. Since the main objective was to verify the correlation observed at the harmonic level, we considered only two systems of Scheme 1 (**1b** and **1c**) and for each of them only the most populated conformer. This approximation was justified by the similarity of the spectra observed at the harmonic level for all different conformers in the CH stretching region (see Figures S12-19

in the Supplementary Materials). The procedure is briefly described in the Computational Details section, while the complete list of NMs is reported in Table S1 of the Supplementary Materials. Interested readers can find a detailed description of the protocol in ref. 56.

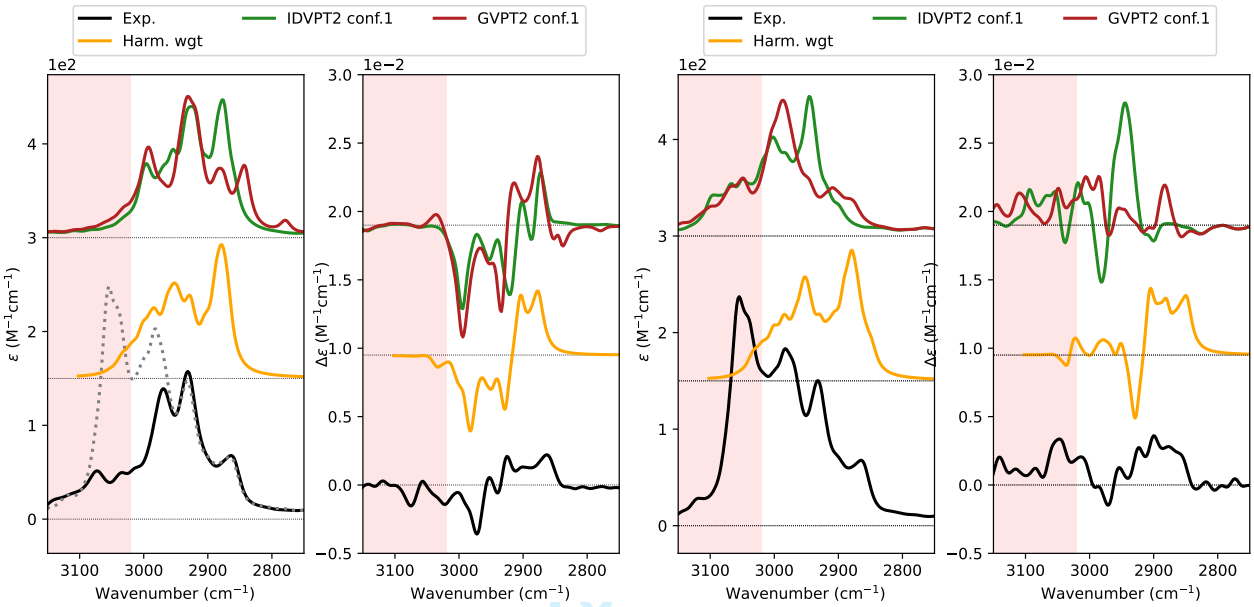


Figure 5: Comparison of experimental IR and VCD spectra in the CH stretching region with scaled harmonic and anharmonic calculated spectra of **1b** and **1c**. In the first panel, the absorption spectra of enantiomer **1a** is drawn in black, while that of **1b** in gray. Experimental VCD spectrum is reported as the semi-difference of the two enantiomers. Only the most populated conformer for either diastereomers is considered. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} half-width at half-maximum. A scaling factor of 0.94 was applied to the harmonic frequencies. The signals of the BPh_4^- counterion, which was not taken into account in the simulations, lay in the portion of the spectra highlighted with a red shade. Harmonic and anharmonic simulated VCD intensities were divided by two to be consistent with order of magnitude of the experimental values.

The results are shown in Figure 5, where we superimpose the experimental VCD spectrum with the scaled harmonic calculations and the IDVPT2 and GVPT2 anharmonic results. Although some differences persist between simulations and experiments, the inclusion of the anharmonic correction does not significantly influence the sign observed for the lowest frequency transitions around 2850 cm^{-1} (see also the simulated harmonic and anharmonic spectra of R_PSS_M-**1** diastereomer, reported in Figure S20 in Supplementary Material). The inclusion of anharmonicity significantly improves the agreement between simulations and ex-

periments for both molecular systems. In particular around 2800 cm^{-1}, the variational correction has a large effect on the overall band-shape,[56] a significant redistribution of the band intensities improving the agreement with the experimental absorption spectra. Nonetheless, the impact of *inactive* modes – not included in the anharmonic subset – on the variational corrections was not systematically investigated and the GVPT2 results need be considered with some care. Far from being a systematic analysis of the impact of anharmonicity in the CH stretching region of this type of complexes, nonetheless, the present results confirm the correlation between the sign of the first VCD band (from low to high wavenumber) and the configuration at the metal center, i.e. $(+)\Leftrightarrow R_M$ and $(-)\Leftrightarrow S_M$.

Conclusions

We have presented the VCD spectra of five quinolinophaneoxazoline-based (η^6-p-cymene) ruthenium(II) half-sandwich complexes and identified the contributions of each molecular moiety, whereever possible. The contributions of the quinolinophane moiety are easy to highlight in the data. More concealed and a little more difficult to pinpoint are the contributions of the external stereocenter located in the oxazoline portion, as well as on the "chiral" ruthenium ion. In fact, from Figure 4 some bands are proposed as signatures for the last two "difficult" cases. Once again we can appreciate here the peculiar value of the VCD in defining local molecular chiral effects, in this sense the VCD can be considered an important almost *sine-qua-non* addition, as in the present case, to OR (in this case) and to the ECD (in general), the latter methods highlighting information on the chirality with a more global or overall character. More specifically, in the present case, OR is noted to be determined by a synergistic effect due to the central chirality of the outer group and the chirality of the metal, while VCD is more specific to the different forms of chirality.

Acknowledgement

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Supporting Information Available

ECD spectra; simulated harmonic spectra of each conformer; Normal modes included in the RD scheme anharmoinc calculations; molecular geometries in XYZ format.

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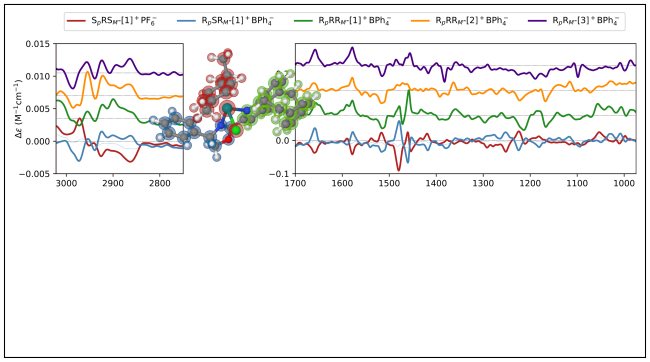
TOC Graphic



Supporting Information: Mid-IR and CH stretching VCD spectroscopy to distinguish various sources of chirality: The case of quinophaneoxazoline based ruthenium(II) complexes

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S1 Additional Experimental Spectra

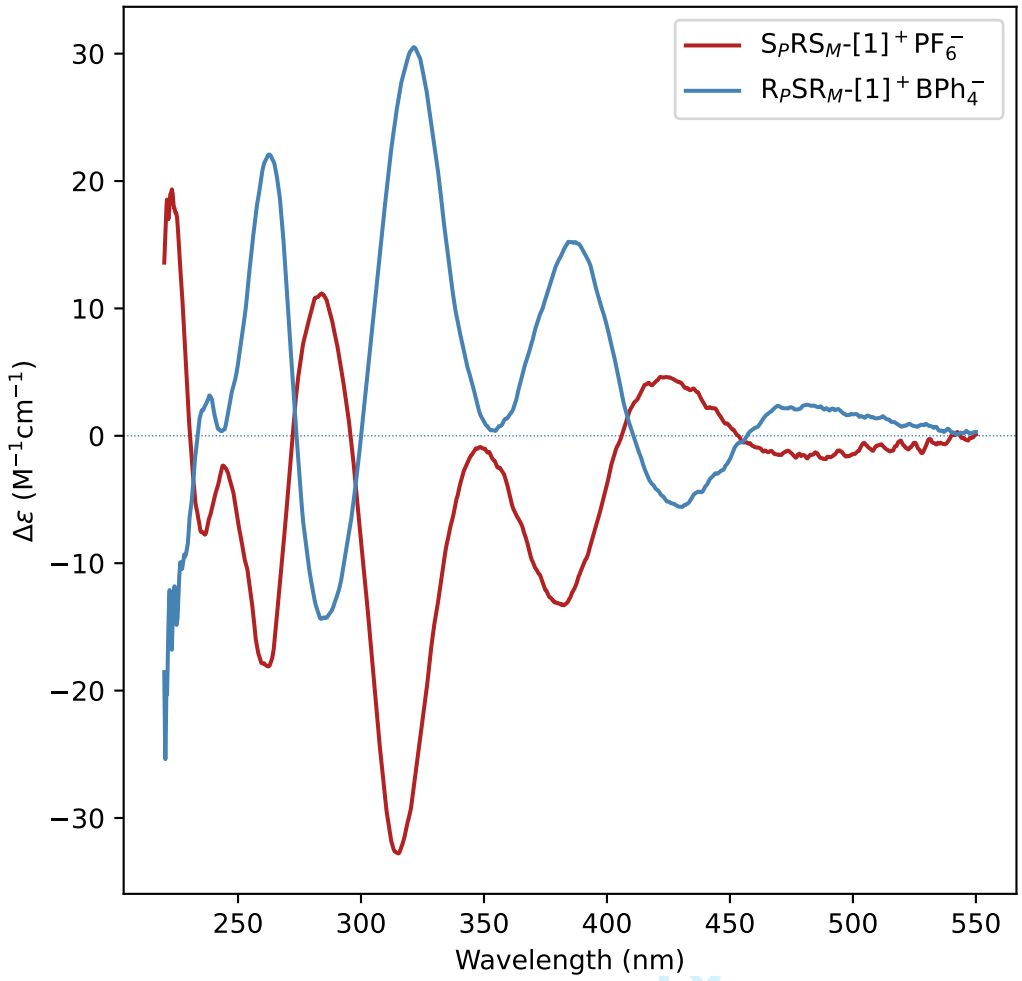

Figure S1: Electronic circular dichroism of R_PSR_M-[1]$^+$ and R_PSR_M-[1]$^+$ recorded in CCl_4 solution.

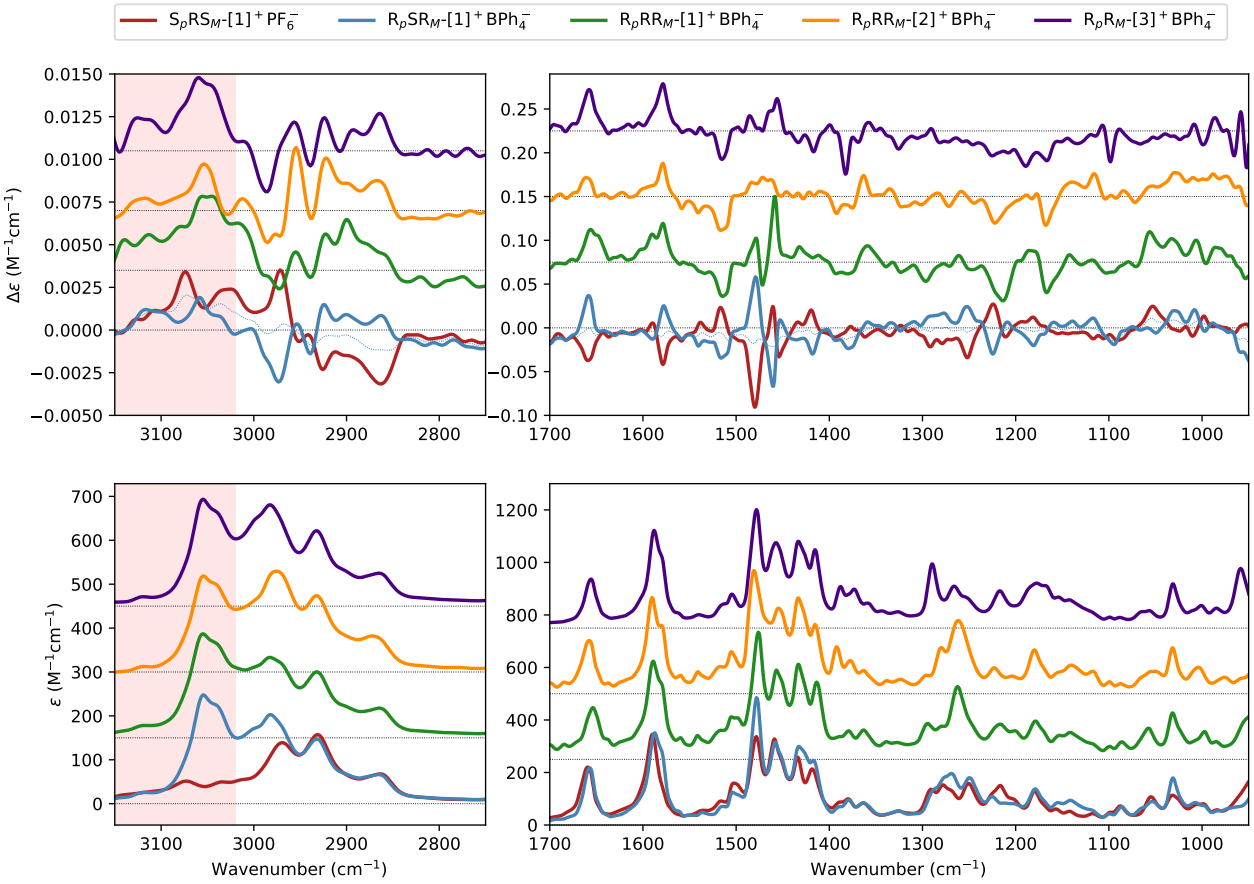

Figure S2: Experimental IR and VCD spectra of ruthenium complexes in the CH-stretching and mid-IR regions. Solvent CCl_4 with 1 mm path length and concentration of $\approx 2.0 \cdot 10^{-2}$M in CH and 200 μm path length and concentration of $\approx 4.0 \cdot 10^{-2}$M in mi.IR region. The portions of the spectra most effected by the presence of the BPh_4 counter ion are highlighted in light red.

S2 Additional Computational Results

Figure S3: Representation of two selected normal modes involved in the first band in the CH-stretching region. On The left the R_p, S, R_M-$[1]^+$ simulated conformer is depicted, whereas on the right the R_p, S, S_M-$[1]^+$ one is reported

S2.1 Additional Simulated Spectra

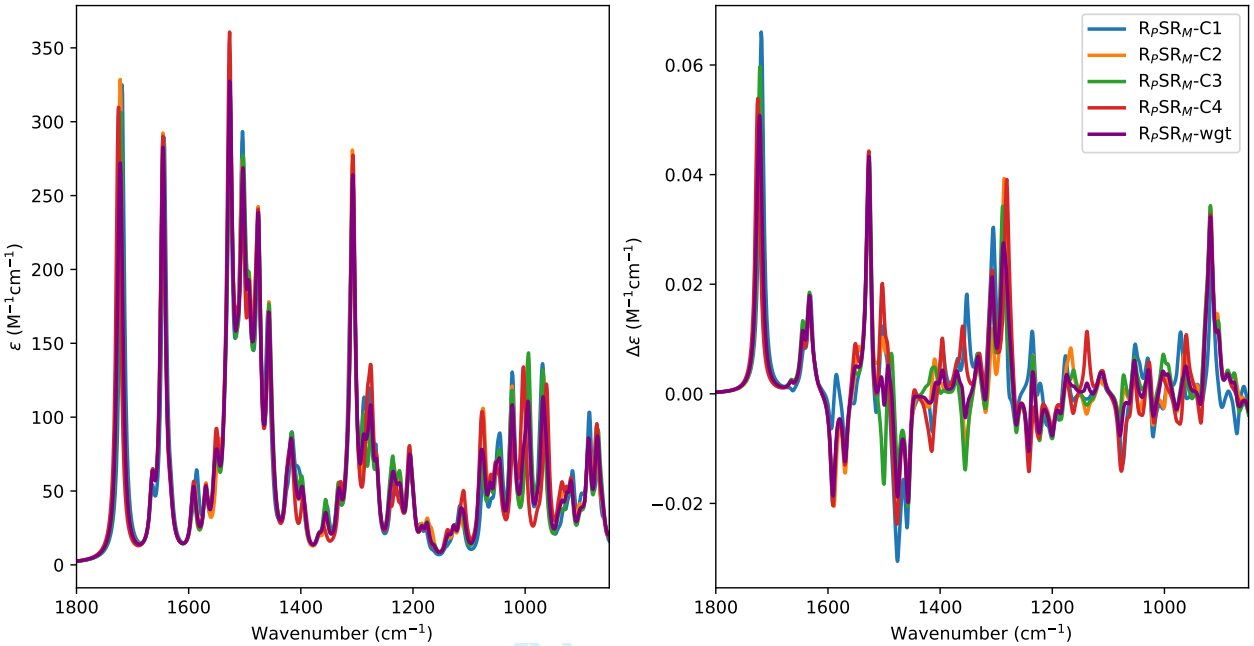

Figure S4: Simulated IR and VCD spectra of each conformer of R_PSR_M-$[1]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

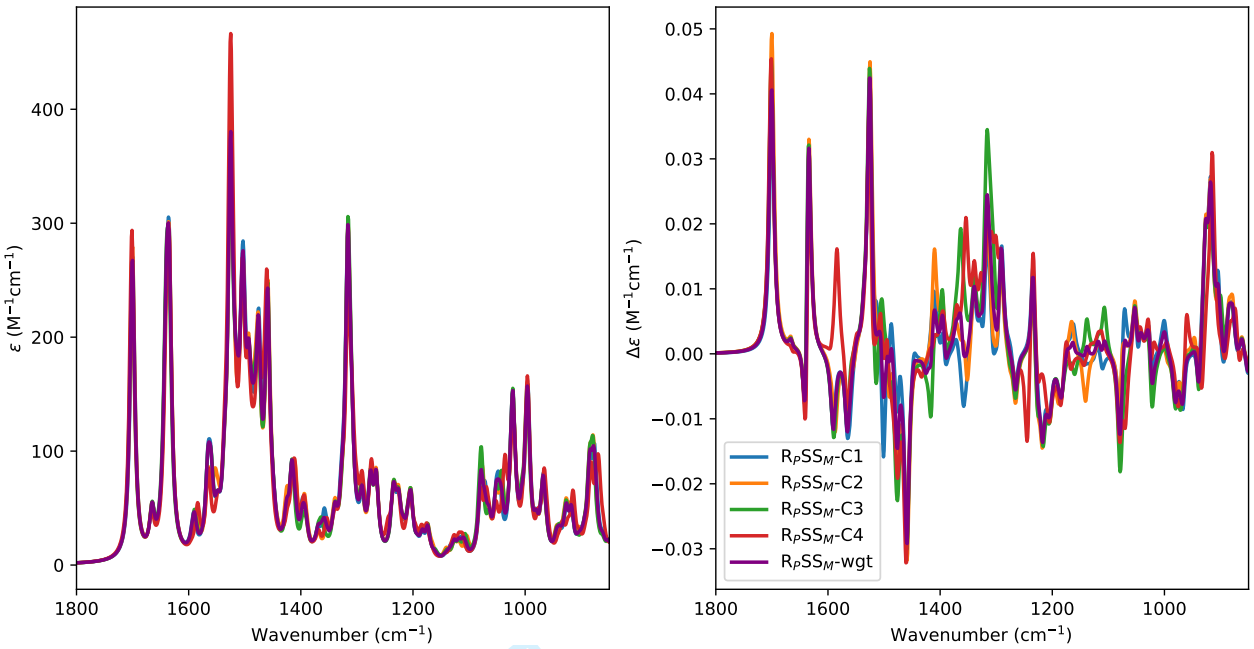

Figure S5: Simulated IR and VCD spectra of each conformer of R_PSS_M-$[1]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

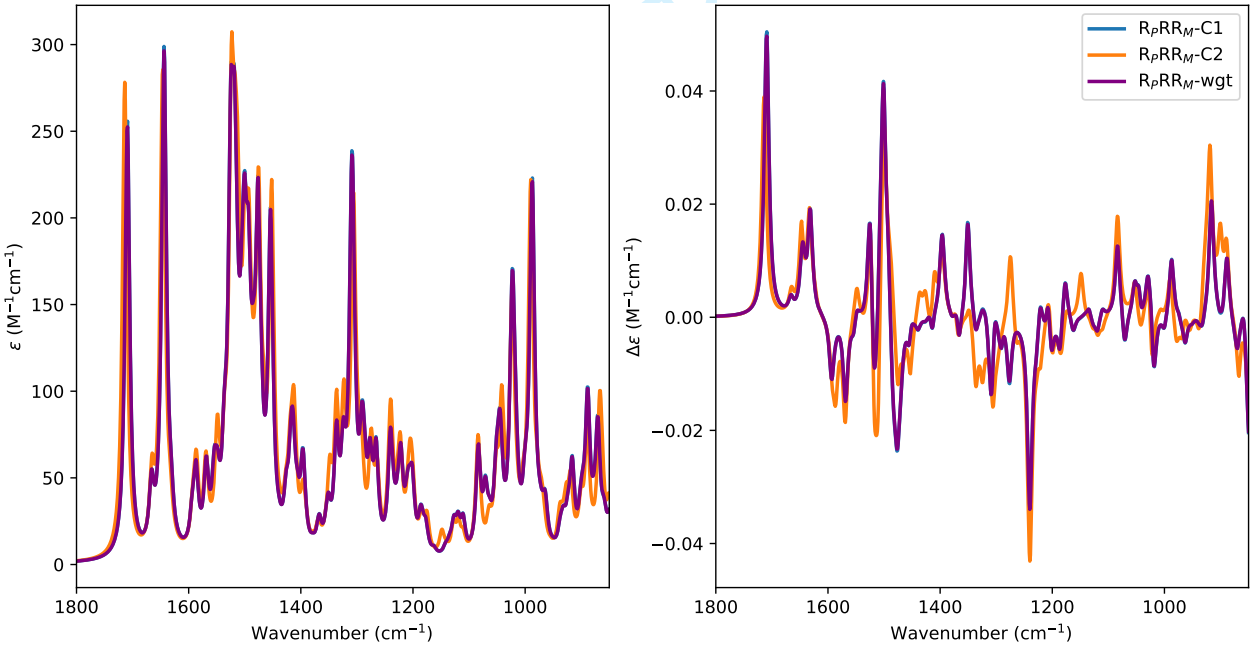

Figure S6: Simulated IR and VCD spectra of each conformer of R_PRR_M-$[1]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

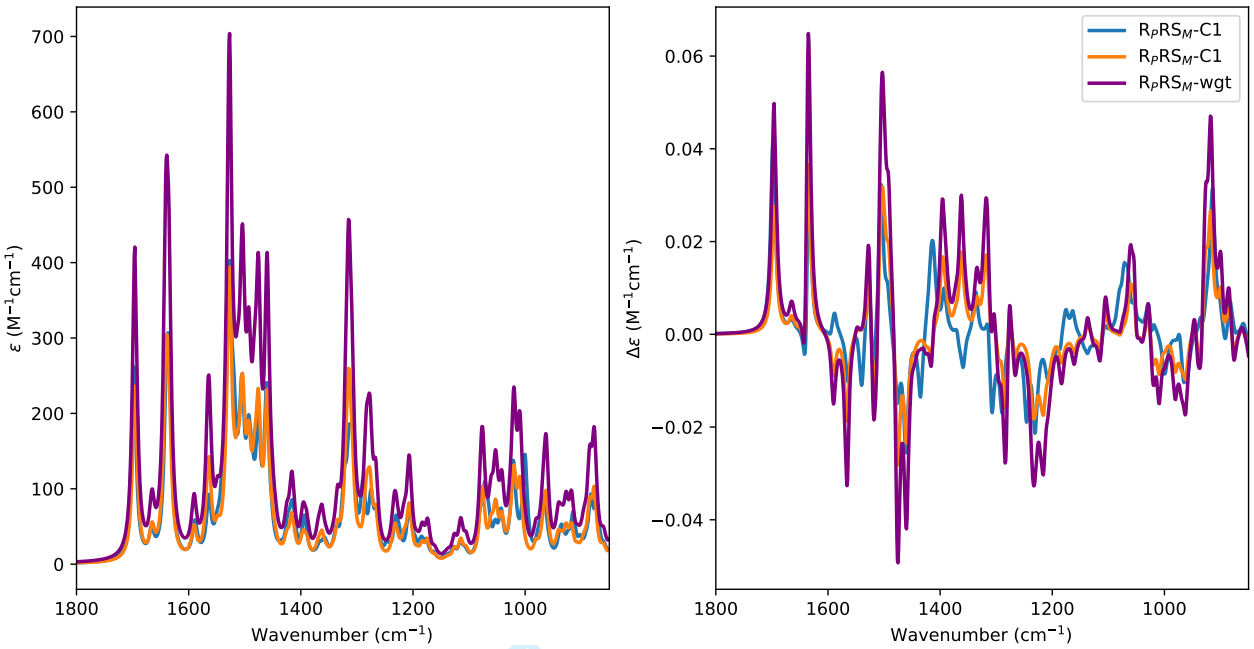

Figure S7: Simulated IR and VCD spectra of each conformer of R_PRS_M-$[1]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying distribution functions with 7 cm^{-1} of half-width at half-maximum.No scaling factor to the harmonic frequencies was applied.

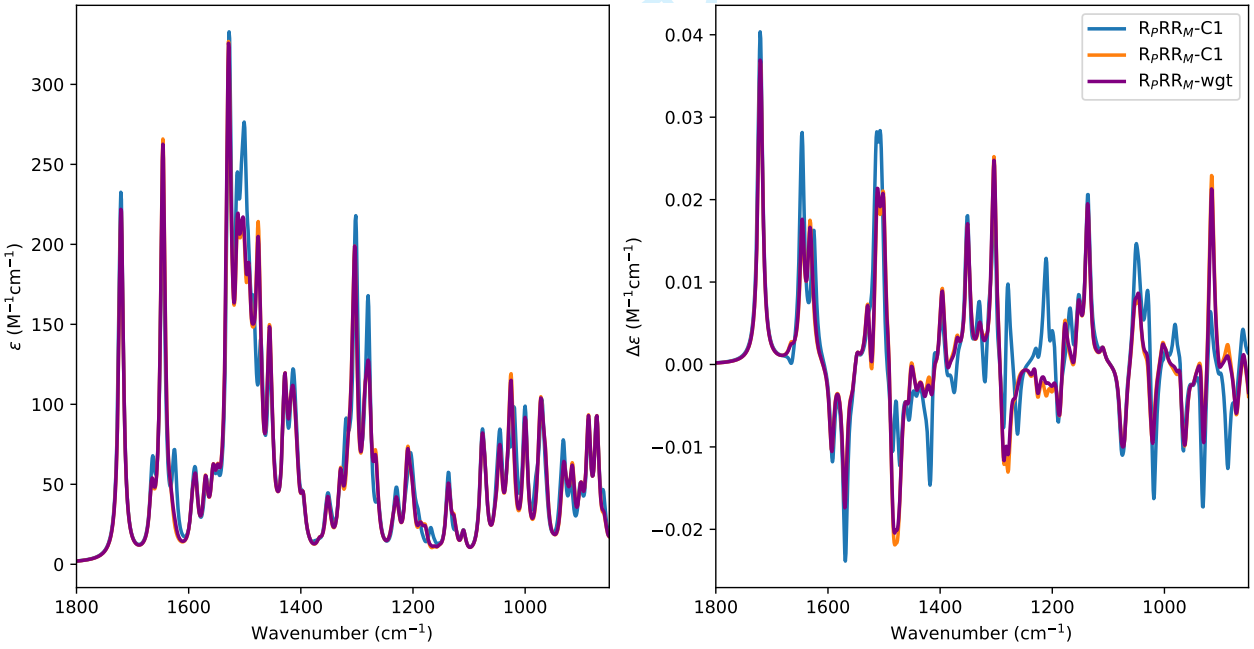

Figure S8: Simulated IR and VCD spectra of each conformer of R_PSR_M-$[2]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

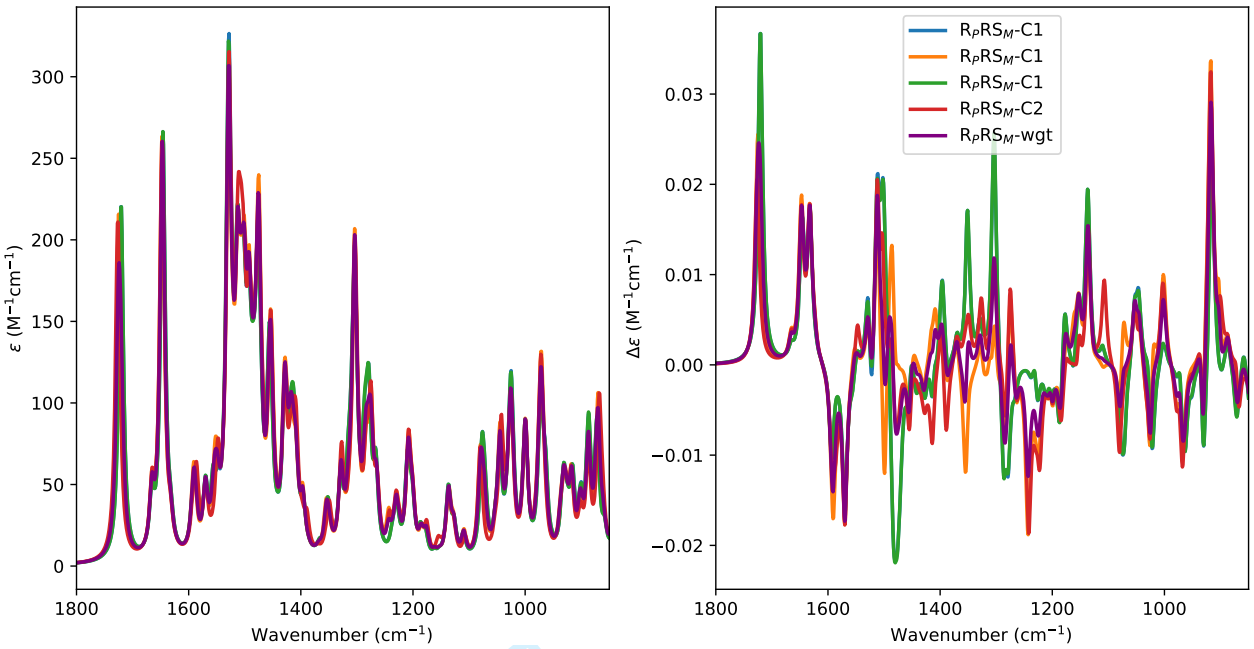

Figure S9: Simulated IR and VCD spectra of each conformer of R_PRS_M-$[2]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

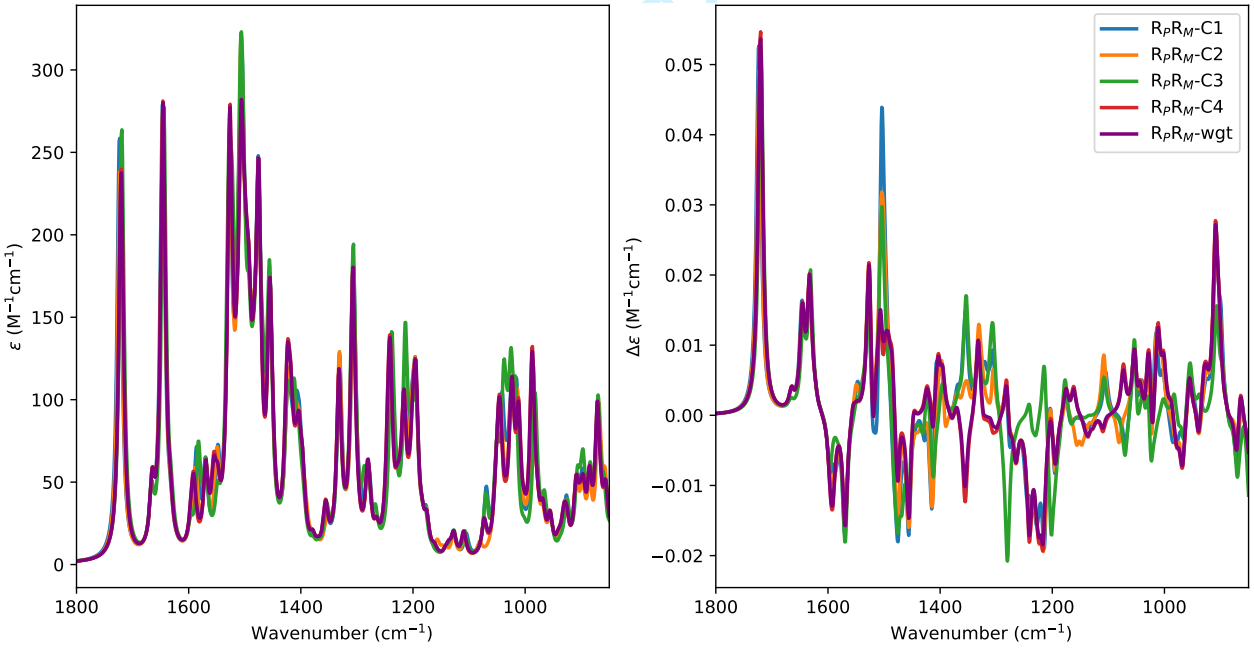

Figure S10: Simulated IR and VCD spectra of each conformer of R_PR_M-$[3]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

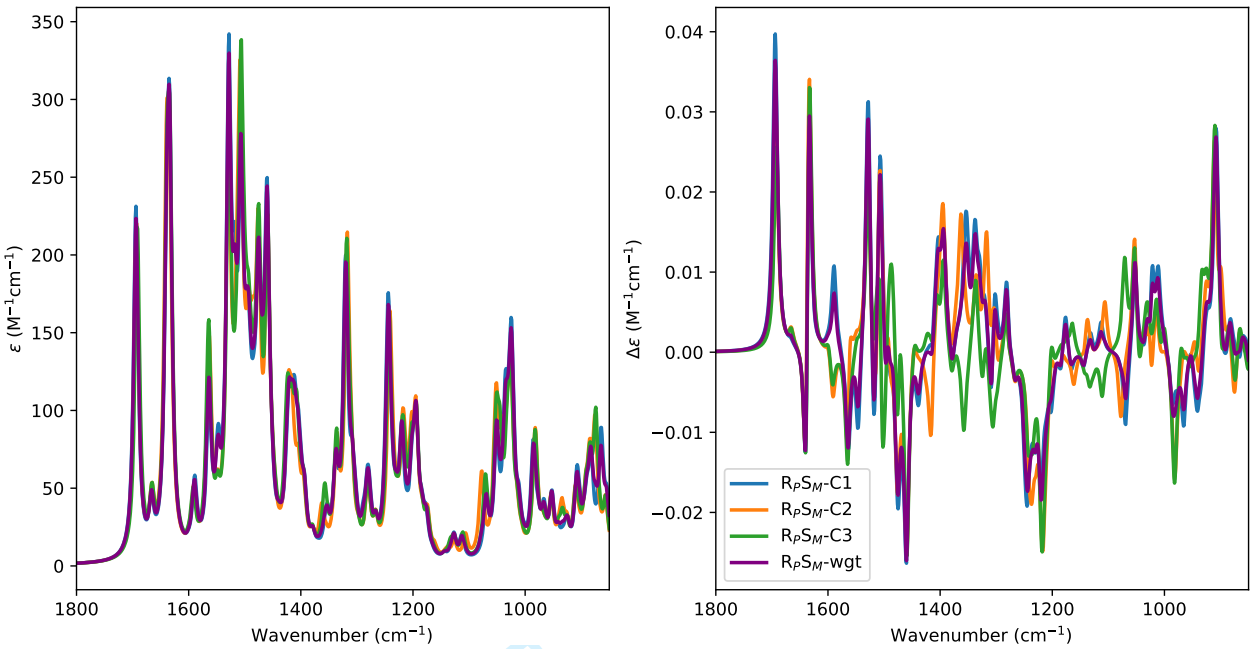

Figure S11: Simulated IR and VCD spectra of each conformer of R_PS_M-$[3]^+$ complex in the mid-IR region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 7 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

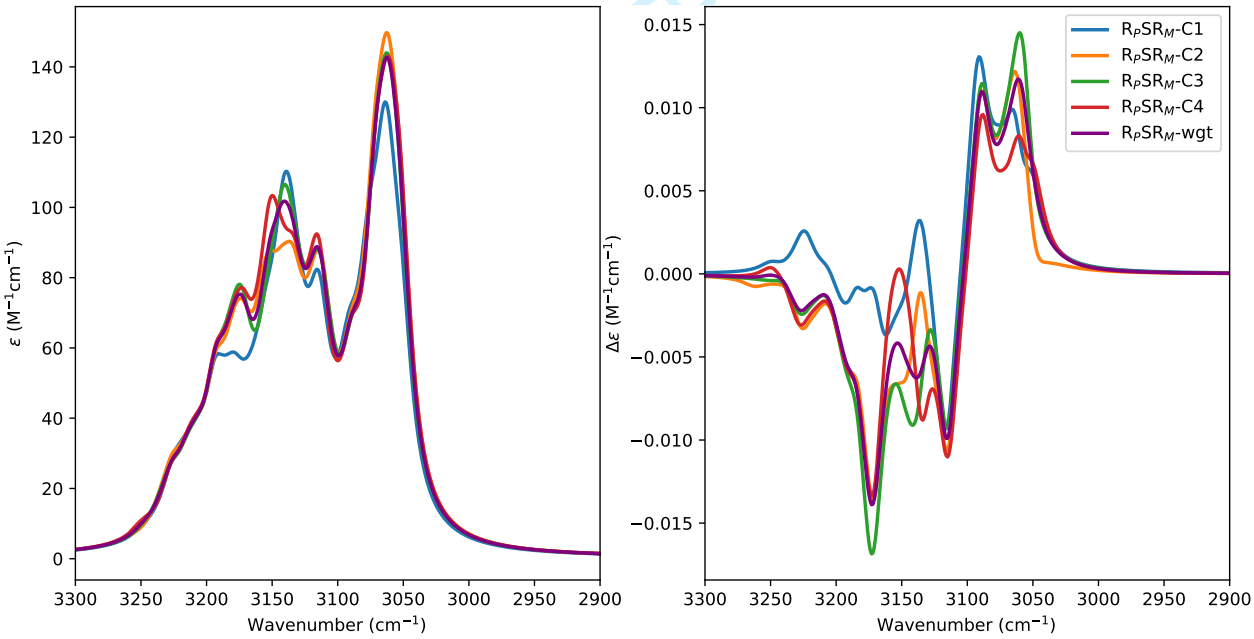

Figure S12: Simulated IR and VCD spectra of each conformer of R_PSR_M-$[1]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

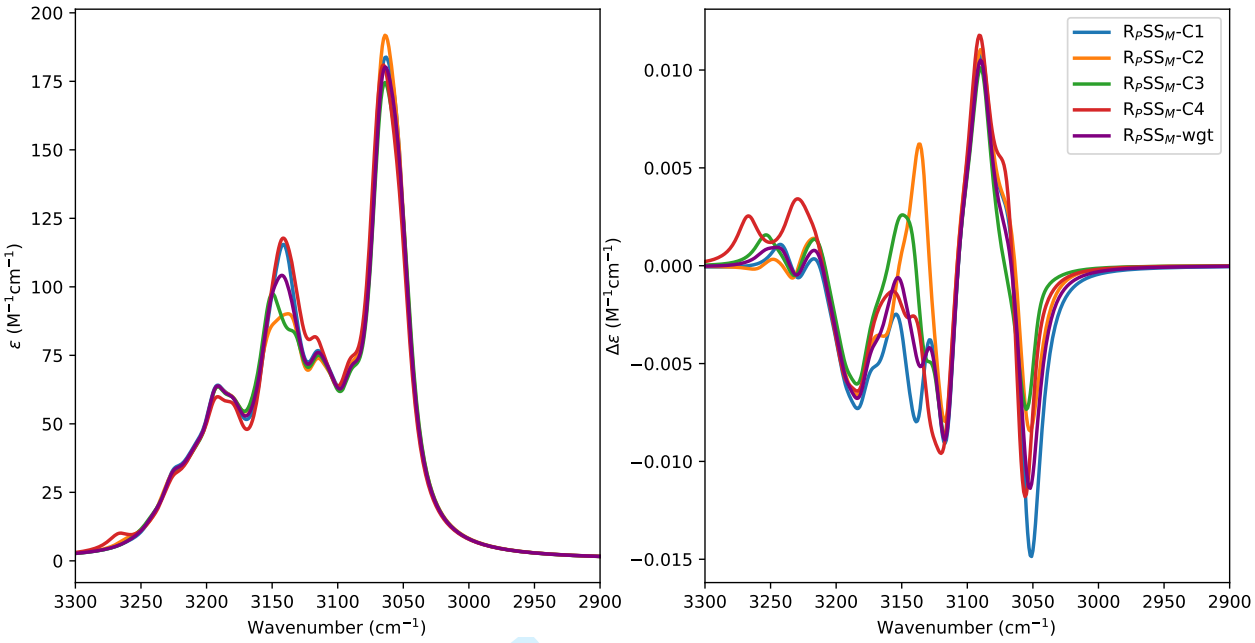

Figure S13: Simulated IR and VCD spectra of each conformer of R_PSS_M-$[1]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

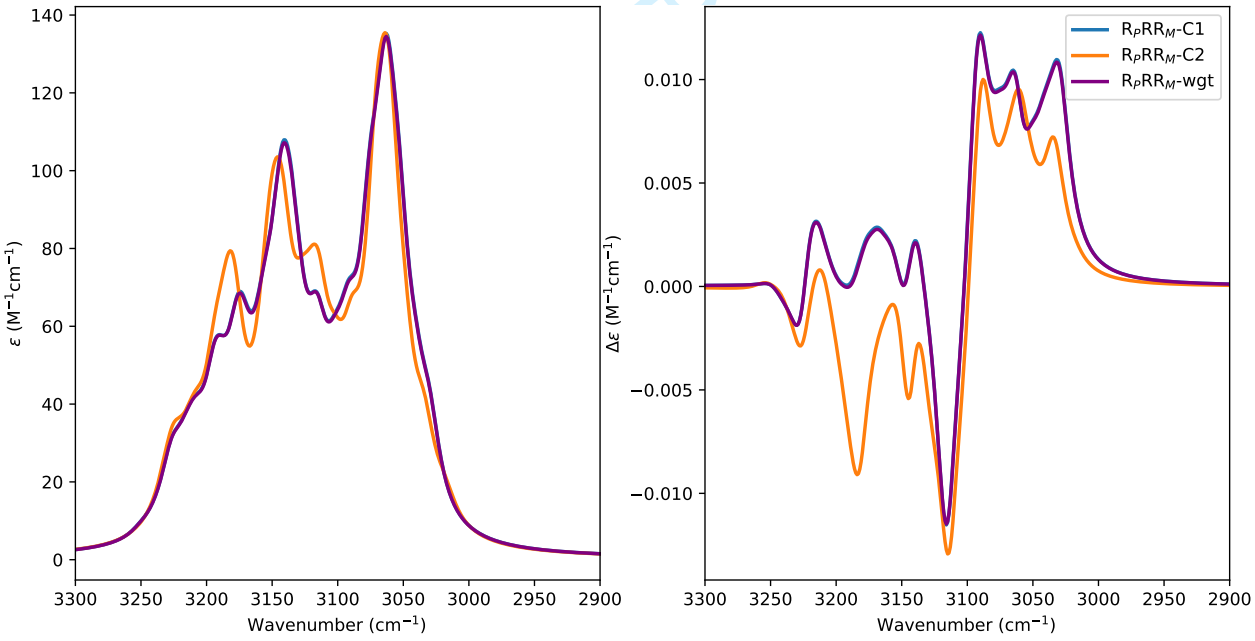

Figure S14: Simulated IR and VCD spectra of each conformer of R_PRR_M-$[1]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

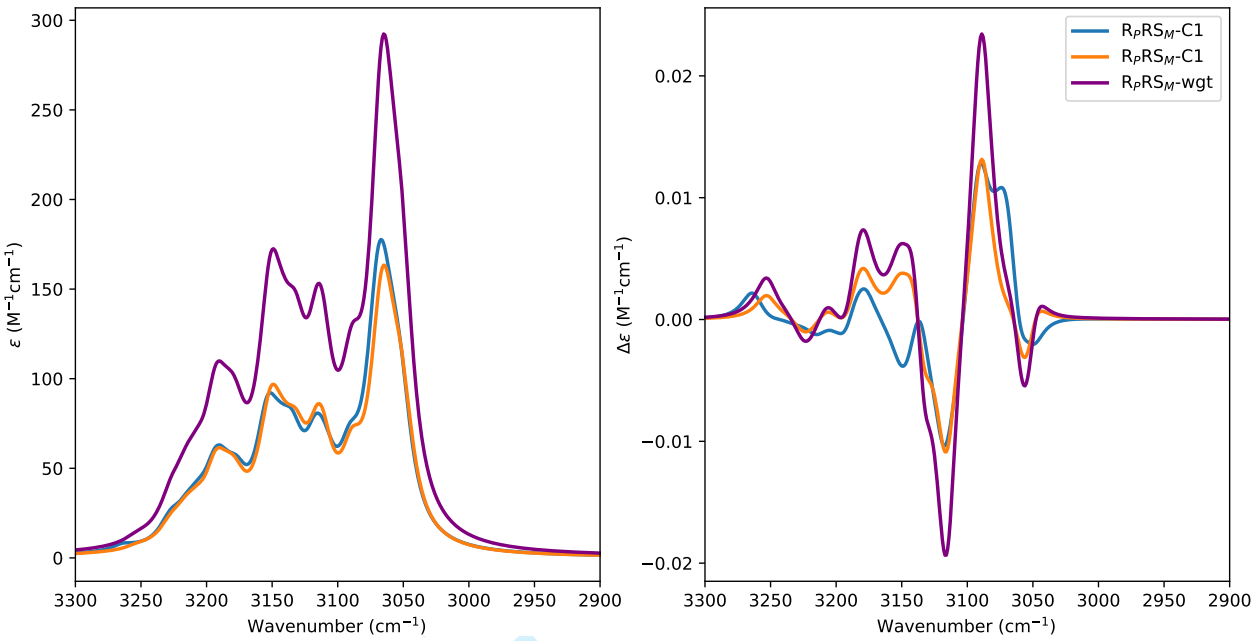

Figure S15: Simulated IR and VCD spectra of each conformer of R_PRS_M-$[1]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

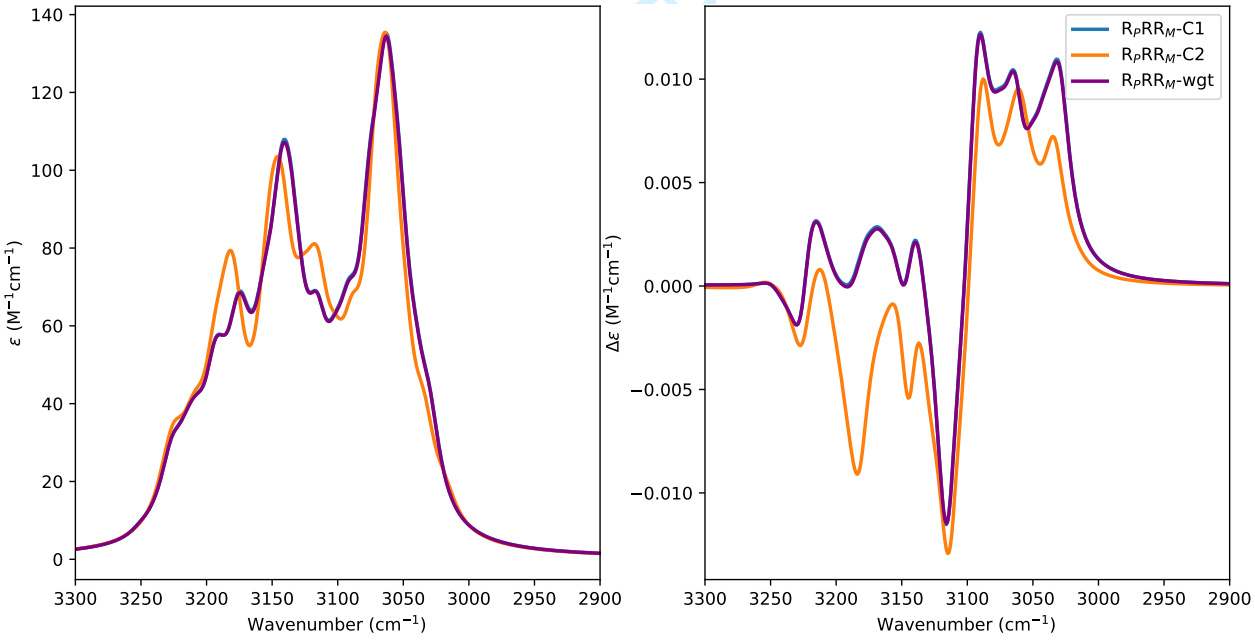

Figure S16: Simulated IR and VCD spectra of each conformer of R_PRR_M-$[2]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

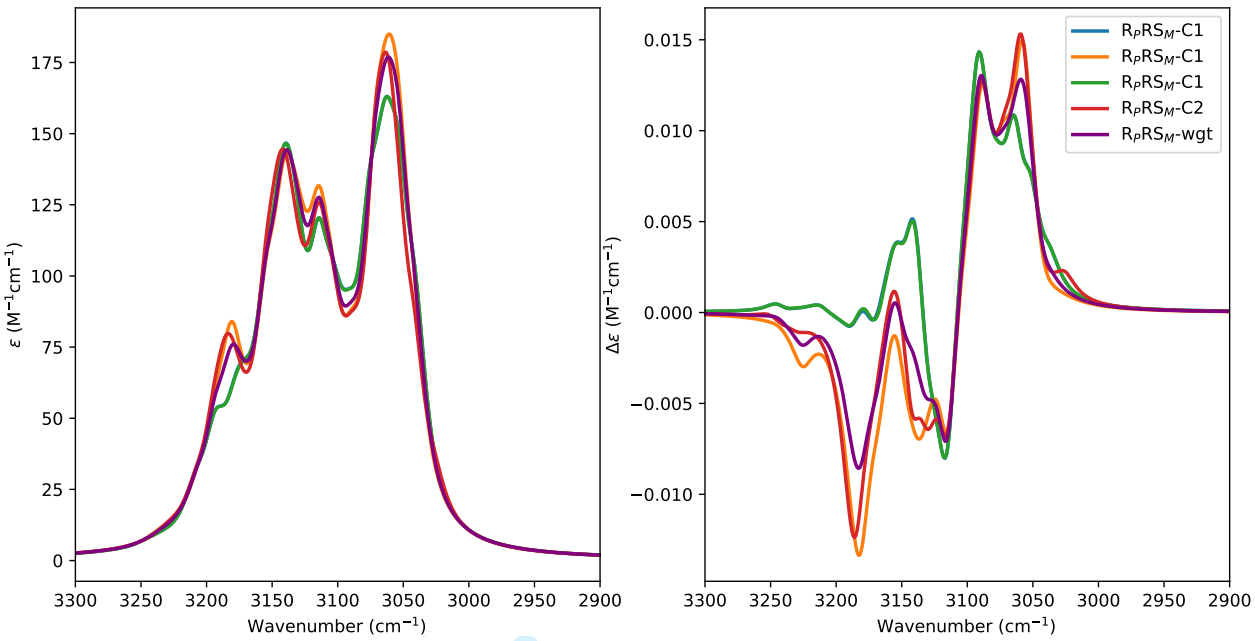

Figure S17: Simulated IR and VCD spectra of each conformer of R_PRS_M-$[2]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

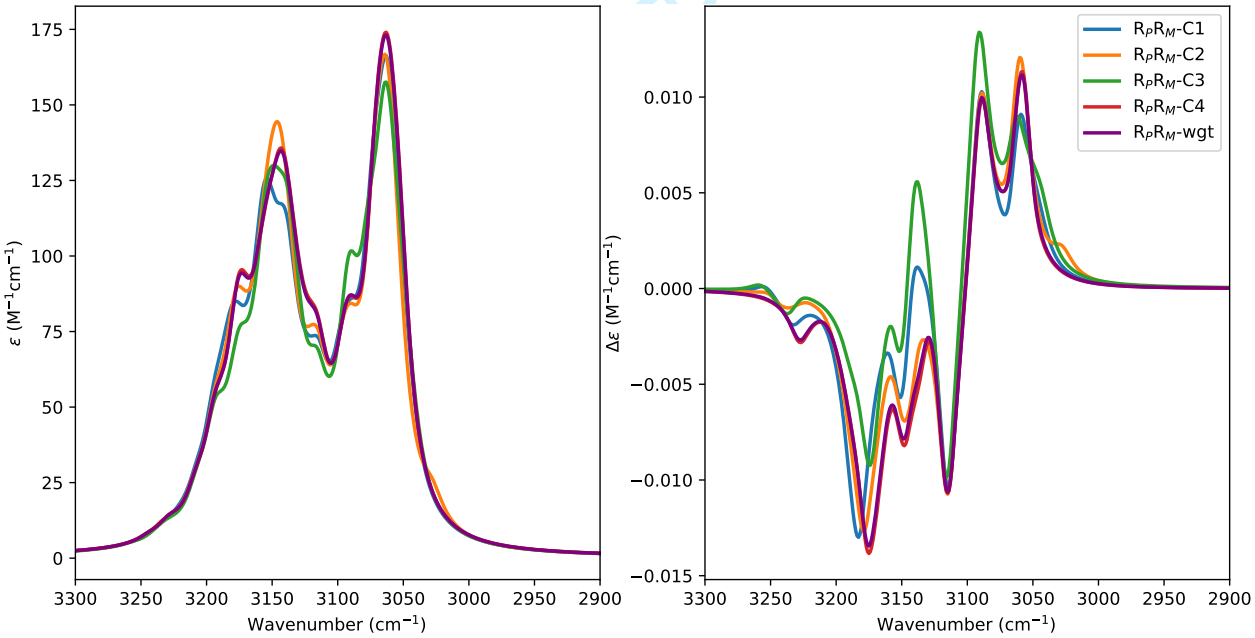

Figure S18: Simulated IR and VCD spectra of each conformer of R_PR_M-$[3]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

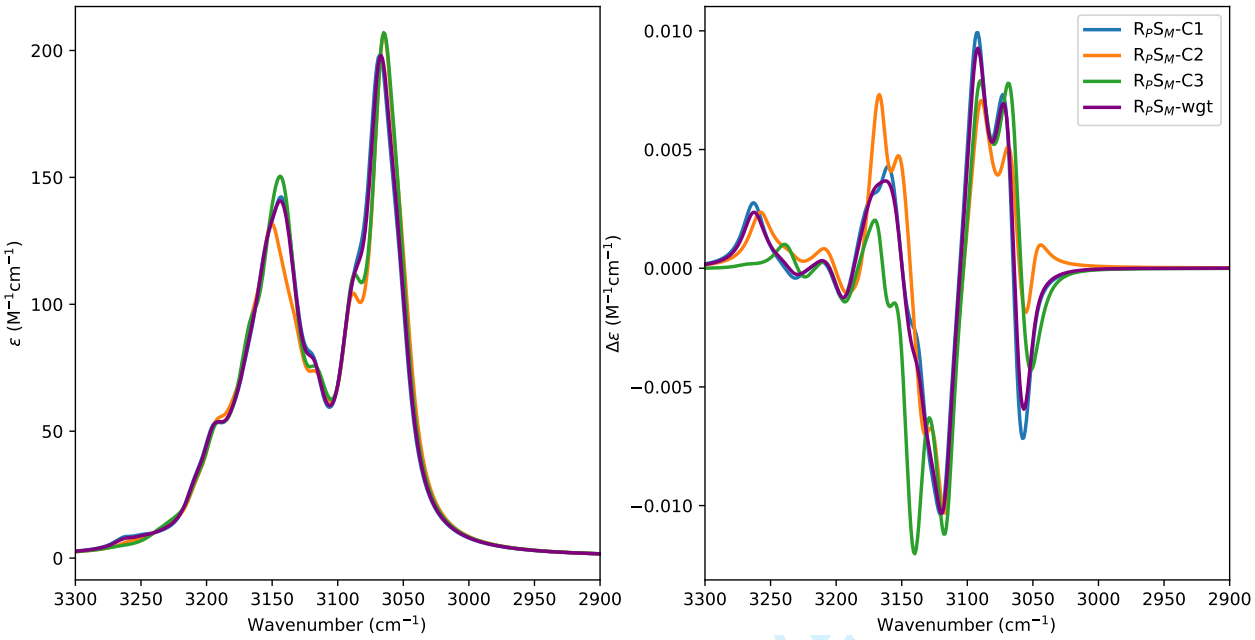

Figure S19: Simulated IR and VCD spectra of each conformer of R_PS_M-$[3]^+$ complex in the CH-stretching region. The calculations were performed at the PW91 level. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} of half-width at half-maximum. No scaling factor to the harmonic frequencies was applied.

S3 Reduced Dimensionality Anharmonic Calculation: the case of two diastereomers with opposite chirality at the metal center.

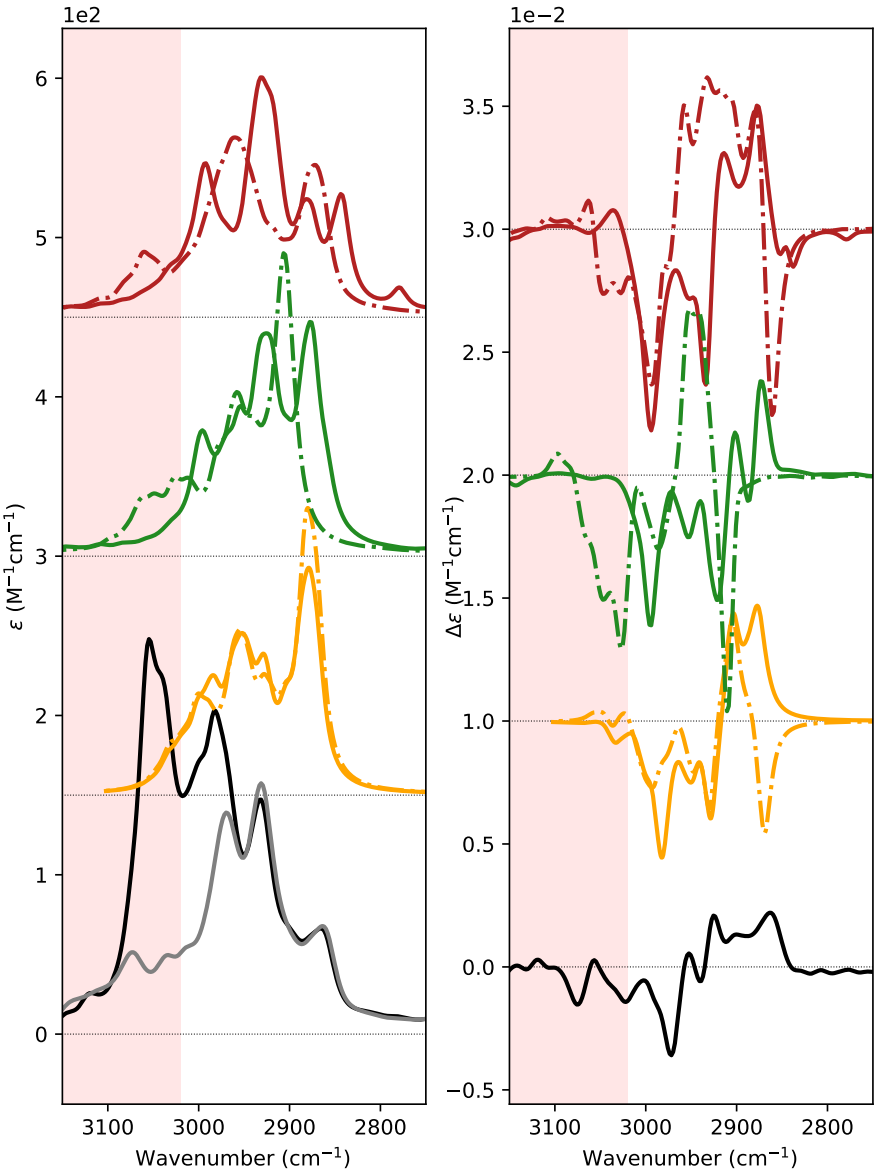

Figure S20: Comparison of experimental IR and VCD spectra of **1** and in the CH stretching region with scaled harmonic and anharmonic calculted spectra. The **1a** absorption spectra is drawn in black, while the **1b** in gray. As experimental VCD the semi-difference of the two enantiomers is reported. The simulated R_PSR_M-**1** are reported as continuous line, while the R_PSS_M-**1** ones as dashed lines. Only the most populated conformer for either diastereomers is considered. The spectral band-shape was obtained by applying Lorentzian distribution functions with 10 cm^{-1} half-width at half-maximum. A 0.94 scaling factor was applied to the harmonic frequencies. BPh_4^- counterion was not taken into account in simulations, its signals lay in the portion of the spectra highlighted with red shade. Harmonic and anharmonic simulated VCD intensities were scaled by two to be consistent with the order of magnitude of the experimental values.

S4 Reduced Dimensionality Anhamronic Calculation Details

Table S1: Normal modes included for each complexes in the spectroscopic region of interest 2750-3150 cm^{-1} in the RD schemes and large amplitude motions (LAM) excluded. A threshold of $\bar{\alpha}_i(j)$=0.015 was used.

Molecule	LAM	NM num.	NMs included
R_PSR_M-[1]$^+$	13	112	58 112 122 123 126 127 145 146 147 148 149 150 151 152 153
	14		154 155 156 157 158 159 160 161 162 163 164 165 166 167 168
	15		169 170 171 172 173 174 175 176 177 178 179 180 181 182 183
	17		184 185 186 187 188 189 190 191 192 193 194 195 196 197 198
	30		199 200 201 202 203 204 205 206 207 208 209 210 211 212 213
	31		214 215 216 217 218 219 220 221 222 223 224 225 226 227 228
	32		229 230 231 232 233 234 235 236 237 238 239 240 241 242 243
	33		244 245 246
R_PRR_M-[1]$^+$	14	102	58 64 74 75 111 123 125 146 148 149 150 151 152 153 154
	15		155 156 157 158 159 160 161 162 163 164 165 166 167 168
	30		169 170 171 172 173 174 175 176 177 178 179 180 181 182
	31		183 184 185 186 187 188 189 190 191 192 193 194 195 196
	32		197 198 199 200 201 202 203 204 205 206 207 208 209 210
	33		211 212 213 214 215 216 217 218 219 220 221 222 223 224
			225 226 227 228 229 230 231 232 233 234 235 236 237 238
			239 240 241 242 243 244 245 246

S5 Cartesian Coordinates

$\mathbf{R}_P\mathbf{SR}_M$-$[\mathbf{1}]^+$: C1

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84
Enegy:  -2248.38548021
C                -4.087100       -0.917415        1.295632
C                -2.302144        1.206153        0.576815
C                -2.815179       -1.243830        0.703579
C                -4.224959        0.358775        1.806370
C                -3.364026        1.406120        1.431225
C                -1.879607       -0.159714        0.402457
H                -5.134079        0.615561        2.343014
H                -3.669564        2.424187        1.662195
C                -1.852426        2.348593       -0.310126
H                -0.933896        2.086145       -0.831928
H                -1.644659        3.233629        0.302644
C                -5.373875       -1.722950        1.179791
H                -6.098272       -1.233553        1.837575
H                -5.298506       -2.750443        1.537731
C                -5.988533       -1.736781       -0.278413
H                -7.077198       -1.800603       -0.173313
H                -5.668573       -2.643356       -0.803825
C                -2.921669        2.783532       -1.406977
H                -2.363716        2.986582       -2.327234
H                -3.385702        3.725470       -1.097772
C                -3.990256        1.745996       -1.625160
C                -5.556583       -0.526135       -1.066021
C                -5.255565        1.877572       -1.039243
C                -3.664390        0.506574       -2.187809
C                -4.438313       -0.615621       -1.904928
C                -6.036347        0.753764       -0.766098
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H                -2.734911        0.393741       -2.742080
H                -4.101580       -1.592761       -2.245359
H                -6.958542        0.869173       -0.200241
C                -2.427466       -2.576860        0.373138
C                -1.226943       -2.756215       -0.288759
H                -0.905859       -3.741761       -0.608632
C                -0.357009       -1.683006       -0.459085
C                -3.199989       -3.815076        0.735511
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H                -2.598886       -4.702426        0.525656
H                -4.128637       -3.908214        0.165731
C                 0.972567       -1.875900       -1.016133
O                 1.257415       -2.931151       -1.770218
C                 2.648048       -2.768869       -2.177395
H                 3.224252       -3.568306       -1.705778
H                 2.685913       -2.871057       -3.262212
C                 3.053340       -1.356728       -1.672554
H                 3.068983       -0.634554       -2.497105
C                 4.383347       -1.325649       -0.957272
C                 6.882778       -1.291702        0.314850
C                 5.443771       -0.591238       -1.496533
C                 4.589060       -2.050947        0.223470
C                 5.829493       -2.031381        0.858325
C                 6.689349       -0.575620       -0.865657
H                 5.296497       -0.031171       -2.417178
H                 3.777014       -2.636372        0.650002
H                 5.979453       -2.599741        1.772000
H                 7.506937       -0.006795       -1.298878
H                 7.851308       -1.282409        0.805994
N                -0.619647       -0.427476       -0.068735
N                 1.892836       -0.997327       -0.834563
Ru                1.260174        0.754326        0.081197
Cl                0.966906        1.404963       -2.224413
C                 1.262231        0.865541        2.361321
C                 2.640041        2.517124        0.413916
C                 0.659814        2.049691        1.813365
C                 2.547565        0.527423        1.890808
C                 3.228990        1.345952        0.933629
C                 1.318327        2.852191        0.868989
H                -0.358520        2.291482        2.098884
H                 3.019724       -0.393123        2.212700
H                 4.194495        1.024501        0.558293
H                 0.808405        3.702835        0.430391
C                 3.333344        3.372857       -0.598371
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H	-0.546267	0.099119	3.125434
C	0.654544	0.777125	4.769477
H	0.309372	1.814926	4.728468
H	1.697951	0.781176	5.102739
H	0.060477	0.256206	5.526506
C	0.938431	-1.395460	3.506004
H	0.278230	-1.925543	4.198439
H	1.957522	-1.500496	3.894207
H	0.882160	-1.899795	2.536172

$\mathbf{R}_P\mathbf{SR}_M$-$[\mathbf{1}]^+$: C2

84
Enegy: -2248.38394767

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C	-4.330058	0.684046	1.636050
C	-3.442125	1.674806	1.178205
C	-1.980961	-0.007368	0.325458
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H	-3.727562	2.715549	1.312874
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H	-0.826438	2.329726	-0.833382
H	-2.031497	3.409388	-0.125301
C	-5.521864	-1.419648	1.197393
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C	-1.376692	-2.659333	-0.154623
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N	-0.718870	-0.338035	-0.090419
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$\mathbf{R}_P\mathbf{SR}_M$-$[\mathbf{1}]^+$: C3

84
Enegy: -2248.38498769

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C	2.685332	-2.549544	-2.308519
H	3.247390	-3.462832	-2.107645
H	2.717177	-2.314004	-3.373645
C	3.114878	-1.355531	-1.405065
H	3.359268	-0.478641	-2.013644

C	4.275742	-1.677396	-0.489542
C	6.471743	-2.335524	1.126966
C	5.509104	-1.047045	-0.677621
C	4.154131	-2.647792	0.513679
C	5.243816	-2.973493	1.318928
C	6.603394	-1.374761	0.125630
H	5.619167	-0.300746	-1.461046
H	3.204257	-3.157038	0.664236
H	5.139736	-3.731193	2.090568
H	7.557820	-0.881990	-0.035441
H	7.322608	-2.594003	1.750284
N	-0.699013	-0.549829	-0.053115
N	1.860856	-1.051176	-0.693898
Ru	1.173795	0.555189	0.426357
Cl	1.072336	1.558823	-1.766962
C	2.470888	2.274679	1.158844
C	1.057392	0.241214	2.673030
C	1.115409	2.473042	1.593080
C	3.079013	1.041791	1.474694
C	2.377425	0.037827	2.217797
C	0.435196	1.486387	2.325498
H	0.598024	3.379675	1.300479
H	4.070867	0.814899	1.102311
H	2.861899	-0.918054	2.387686
H	-0.606783	1.639201	2.586589
C	0.321547	-0.790127	3.473942
H	-0.738707	-0.818681	3.209443
H	0.390407	-0.547596	4.541131
H	0.745627	-1.786717	3.330149
C	3.163091	3.381351	0.396560
H	2.411217	3.800139	-0.283935
C	4.348649	2.922505	-0.448892
H	4.048829	2.144373	-1.156209
H	5.176360	2.553897	0.167701
H	4.730828	3.767861	-1.028093
C	3.579835	4.476330	1.396809
H	2.730998	4.850748	1.977839
H	4.013862	5.323186	0.857037
H	4.332807	4.102875	2.099398

$\mathbf{R}_P\mathbf{SR}_M$-$[\mathbf{1}]^+$: C4

84
Enegy: -2248.38386315

C	-4.334992	-1.142191	0.936307
C	-2.439268	0.994180	0.705522
C	-3.021875	-1.426210	0.416766
C	-4.488043	0.049032	1.619054
C	-3.570110	1.106406	1.484091
C	-2.036935	-0.345562	0.363808
H	-5.436367	0.258277	2.106217
H	-3.869269	2.089735	1.840012
C	-1.878155	2.237134	0.047854
H	-0.917159	2.022806	-0.416603
H	-1.715309	3.012399	0.805466
C	-5.624943	-1.871309	0.586595
H	-6.395098	-1.457742	1.244432
H	-5.608720	-2.942758	0.789539
C	-6.100927	-1.644241	-0.905525
H	-7.195952	-1.679099	-0.907899
H	-5.757459	-2.475299	-1.531364
C	-2.823670	2.867254	-1.068583
H	-2.174192	3.175124	-1.894829
H	-3.288578	3.774336	-0.669567
C	-3.894572	1.916524	-1.532602
C	-5.565553	-0.348882	-1.460624
C	-5.204964	2.010971	-1.047158
C	-3.550927	0.761289	-2.244162
C	-4.377272	-0.358414	-2.202360
C	-6.037090	0.891252	-1.015467
H	-5.538866	2.935291	-0.580204
H	-2.577316	0.694059	-2.725248
H	-4.036550	-1.287387	-2.655142
H	-7.004514	0.959041	-0.522065
C	-2.636844	-2.710058	-0.073131
C	-1.384044	-2.835862	-0.644300

H	-1.057812	-3.775792	-1.076497
C	-0.477873	-1.781210	-0.577801
C	-3.470197	-3.957519	0.029577
H	-3.824444	-4.116175	1.051750
H	-2.874294	-4.826911	-0.256441
H	-4.343179	-3.929792	-0.628364
C	0.893210	-1.939683	-1.036861
O	1.220764	-2.881290	-1.913721
C	2.643980	-2.707625	-2.177243
H	3.158775	-3.595013	-1.802128
H	2.769869	-2.631787	-3.257665
C	3.040773	-1.412824	-1.414985
H	3.162130	-0.572120	-2.107664
C	4.293085	-1.558627	-0.582334
C	6.657226	-1.854122	0.898370
C	5.420690	-0.789413	-0.884892
C	4.363523	-2.484740	0.466565
C	5.536334	-2.629521	1.205240
C	6.598851	-0.937201	-0.150170
H	5.379806	-0.074380	-1.703462
H	3.499205	-3.101137	0.706297
H	5.581244	-3.353442	2.014093
H	7.470070	-0.339046	-0.401008
H	7.573559	-1.972844	1.468982
N	-0.746756	-0.586413	-0.033389
N	1.814080	-1.134625	-0.642796
Ru	1.143360	0.491441	0.463445
Cl	1.103682	1.464910	-1.745936
C	2.450964	2.196745	1.233928
C	1.004499	0.152767	2.704300
C	1.098364	2.405613	1.660126
C	3.037327	0.944109	1.526714
C	2.325498	-0.060165	2.255282
C	0.400502	1.407952	2.365140
H	0.588353	3.320475	1.388304
H	4.031178	0.718472	1.154975
H	2.797128	-1.024081	2.414899
H	-0.642212	1.569245	2.618755
C	0.250712	-0.880458	3.485879
H	-0.808931	-0.888926	3.217641
H	0.319487	-0.656883	4.557186
H	0.660129	-1.880908	3.326688
C	3.255036	3.252486	0.501816
H	3.738442	2.743008	-0.341506
C	4.353586	3.778576	1.445352
H	5.008937	2.979852	1.805960
H	3.917245	4.278776	2.316905
H	4.973601	4.509449	0.917662
C	2.423524	4.406097	-0.058483
H	1.631455	4.046279	-0.719874
H	3.069926	5.067533	-0.642356
H	1.983751	5.014317	0.740828

$\mathbf{R}_P\mathbf{SS}_M$-$[\mathbf{1}]^+$: C1

84
Enegy: -2248.37433088

C	-4.193448	-0.937061	1.233148
C	-2.446332	1.227039	0.575972
C	-2.947919	-1.222035	0.569475
C	-4.318340	0.309601	1.818732
C	-3.485318	1.388335	1.463356
C	-2.027763	-0.122177	0.325945
H	-5.208007	0.527438	2.402999
H	-3.799912	2.390475	1.745944
C	-2.013623	2.367364	-0.323943
H	-1.171230	2.027422	-0.928224
H	-1.676709	3.231394	0.259862
C	-5.477089	-1.748077	1.130358
H	-6.170837	-1.316304	1.857756
H	-5.367344	-2.795883	1.413096
C	-6.172626	-1.677149	-0.291141
H	-7.254404	-1.738769	-0.130014
H	-5.891845	-2.555357	-0.882533
C	-3.152395	2.894473	-1.297418
H	-2.665129	3.205438	-2.229043

H	-3.601178	3.793344	-0.862713
C	-4.231126	1.871049	-1.540499
C	-5.776106	-0.427556	-1.035122
C	-5.469536	1.970996	-0.894534
C	-3.935727	0.664424	-2.184454
C	-4.699133	-0.471334	-1.929976
C	-6.240320	0.834596	-0.648599
H	-5.777360	2.923966	-0.469233
H	-3.033056	0.576446	-2.786016
H	-4.379550	-1.428358	-2.336686
H	-7.135006	0.919562	-0.035514
C	-2.573899	-2.514235	0.087307
C	-1.413243	-2.619214	-0.657819
H	-1.105777	-3.569045	-1.081293
C	-0.536599	-1.538473	-0.727697
C	-3.318298	-3.787031	0.378727
H	-4.285445	-3.833623	-0.129297
H	-3.494683	-3.899564	1.452048
H	-2.731815	-4.645977	0.046147
C	0.807324	-1.695516	-1.261233
O	1.091414	-2.657703	-2.131803
C	2.533877	-2.610821	-2.315132
H	2.960862	-3.471681	-1.793987
H	2.737183	-2.678731	-3.383889
C	2.969754	-1.266534	-1.676531
H	3.108962	-0.503769	-2.453496
C	4.245262	-1.384350	-0.877724
C	6.658075	-1.687187	0.512366
C	5.443627	-0.916232	-1.427761
C	4.261596	-2.009203	0.375666
C	5.463902	-2.154432	1.066232
C	6.647215	-1.069178	-0.737551
H	5.441659	-0.436129	-2.404615
H	3.333061	-2.355089	0.824029
H	5.467790	-2.636801	2.039631
H	7.572185	-0.707272	-1.176956
H	7.592858	-1.807587	1.052053
N	-0.780771	-0.335885	-0.195331
N	1.758381	-0.898651	-0.909080
Ru	1.240029	0.444424	0.596362
Cl	0.975695	-1.525844	1.973551
C	2.464502	2.244067	-0.142656
C	1.459320	1.652386	2.523977
C	3.205378	1.424149	0.772399
C	1.199350	2.689307	0.287016
C	0.707427	2.397516	1.600580
C	2.713867	1.125847	2.059612
H	4.139149	0.974347	0.451242
H	0.576921	3.256924	-0.392305
H	-0.287483	2.722848	1.882174
H	3.266490	0.438612	2.691070
C	0.963320	1.346902	3.901147
H	1.096383	0.286480	4.131374
H	-0.094649	1.594989	4.007802
H	1.531331	1.934312	4.632103
C	3.061148	2.609562	-1.484281
H	3.724236	1.782038	-1.767602
C	3.938895	3.862815	-1.311374
H	4.440516	4.102758	-2.253841
H	4.708802	3.718211	-0.547248
H	3.332526	4.727960	-1.022322
C	2.032167	2.801834	-2.599247
H	2.543948	2.939706	-3.556181
H	1.418130	3.694587	-2.438709
H	1.366668	1.937461	-2.690505

$\mathbf{R}_P\mathbf{SS}_M$-$[\mathbf{1}]^+$: C2

84
Enegy: -2248.37052835

C	-4.202069	-0.910911	1.214589
C	-2.498370	1.273030	0.509827
C	-2.954335	-1.183519	0.550455
C	-4.352281	0.346306	1.771992
C	-3.542273	1.433385	1.392222
C	-2.054553	-0.071865	0.286944

H	-5.244629	0.557737	2.354668
H	-3.872249	2.435421	1.656866
C	-2.080709	2.408679	-0.398270
H	-1.126769	2.161915	-0.867410
H	-1.945476	3.324698	0.187437
C	-5.467570	-1.753642	1.142118
H	-6.161691	-1.324817	1.870737
H	-5.327762	-2.792238	1.444533
C	-6.185089	-1.728912	-0.271996
H	-7.265248	-1.758555	-0.092768
H	-5.934000	-2.638941	-0.827461
C	-3.128796	2.762065	-1.550695
H	-2.564201	2.887396	-2.481157
H	-3.577492	3.733296	-1.320065
C	-4.212234	1.730430	-1.710402
C	-5.775762	-0.522865	-1.077815
C	-5.445625	1.877274	-1.062954
C	-3.931466	0.488609	-2.290390
C	-4.706049	-0.624403	-1.975843
C	-6.223677	0.762683	-0.752122
H	-5.744236	2.855320	-0.691537
H	-3.034420	0.362471	-2.893490
H	-4.400277	-1.604120	-2.336378
H	-7.114300	0.887326	-0.139915
C	-2.560799	-2.473703	0.076098
C	-1.406520	-2.563718	-0.679834
H	-1.087778	-3.510935	-1.100914
C	-0.543921	-1.470775	-0.755496
C	-3.279946	-3.757045	0.383649
H	-4.253416	-3.822102	-0.109974
H	-3.438932	-3.866788	1.460029
H	-2.684073	-4.607989	0.047164
C	0.805742	-1.618120	-1.277269
O	1.103375	-2.558289	-2.166746
C	2.546918	-2.498766	-2.341455
H	2.973577	-3.384564	-1.864239
H	2.753275	-2.512800	-3.411828
C	2.980130	-1.185907	-1.636141
H	3.154892	-0.394024	-2.375623
C	4.225589	-1.348394	-0.797581
C	6.585348	-1.733895	0.662268
C	5.433325	-0.802908	-1.245347
C	4.205756	-2.090193	0.390614
C	5.381278	-2.278433	1.115631
C	6.610532	-0.995516	-0.520174
H	5.460468	-0.233332	-2.172600
H	3.268096	-2.494249	0.764863
H	5.357003	-2.853800	2.036788
H	7.543493	-0.572637	-0.881241
H	7.499961	-1.888142	1.227358
N	-0.802838	-0.269499	-0.229053
N	1.752298	-0.833064	-0.890077
Ru	1.242894	0.485270	0.631744
Cl	0.893663	-1.496473	1.961134
C	1.819242	2.620424	-0.032417
C	2.226634	1.299656	2.526463
C	2.954202	1.805816	0.210735
C	0.852705	2.661944	1.013056
C	1.039368	2.032910	2.267935
C	3.162065	1.157750	1.463227
H	3.682030	1.640477	-0.576121
H	-0.072744	3.194881	0.840602
H	0.257270	2.078174	3.017381
H	4.028574	0.519830	1.595049
C	2.466732	0.656835	3.853378
H	3.082344	-0.238658	3.759316
H	1.529882	0.381069	4.339795
H	2.993939	1.376532	4.492814
C	1.636957	3.436401	-1.294306
H	0.562185	3.633671	-1.392209
C	2.099329	2.728188	-2.569263
H	1.850813	3.337112	-3.443375
H	1.611324	1.755362	-2.683990
H	3.184934	2.580880	-2.584313
C	2.344640	4.792486	-1.121804
H	2.163048	5.426583	-1.995059
H	3.427532	4.660001	-1.021528
H	1.987126	5.327046	-0.236320

$\mathbf{R}_P\mathbf{SS}_M$-$[\mathbf{1}]^+$: C3

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84
Enegy:  -2248.37397066
C                  -4.175506       -0.974244        1.273663
C                  -2.431954        1.201956        0.650723
C                  -2.933251       -1.245977        0.598799
C                  -4.297326        0.260274        1.885013
C                  -3.465136        1.344953        1.547922
C                  -2.014596       -0.141104        0.367837
H                  -5.183939        0.466673        2.478035
H                  -3.775361        2.341073        1.855158
C                  -2.005235        2.362936       -0.224174
H                  -1.175728        2.031652       -0.850461
H                  -1.652427        3.207802        0.378046
C                  -5.460531       -1.781378        1.158014
H                  -6.151984       -1.363198        1.895515
H                  -5.352379       -2.834989        1.418871
C                  -6.158631       -1.680141       -0.260108
H                  -7.239830       -1.751139       -0.098760
H                  -5.874149       -2.542598       -0.872560
C                  -3.154601        2.921732       -1.165911
H                  -2.677914        3.266236       -2.091314
H                  -3.600950        3.803846       -0.695796
C                  -4.233210        1.903444       -1.431477
C                  -5.769273       -0.411438       -0.975034
C                  -5.468934        1.984010       -0.777779
C                  -3.937487        0.713735       -2.106071
C                  -4.696191       -0.430184       -1.875518
C                  -6.235539        0.839657       -0.556319
H                  -5.777178        2.925210       -0.327303
H                  -3.037131        0.642827       -2.713356
H                  -4.375480       -1.376148       -2.306518
H                  -7.127642        0.907216        0.062681
C                  -2.561989       -2.530242        0.094555
C                  -1.406543       -2.622003       -0.659525
H                  -1.100293       -3.564855       -1.099166
C                  -0.533605       -1.537641       -0.723599
C                  -3.303498       -3.808084        0.371188
H                  -4.271349       -3.849925       -0.136022
H                  -3.478034       -3.935055        1.443162
H                  -2.715999       -4.661466        0.026252
C                   0.801445       -1.688147       -1.279332
O                   1.068817       -2.639929       -2.166751
C                   2.507478       -2.593704       -2.374801
H                   2.941811       -3.462363       -1.873042
H                   2.691996       -2.647305       -3.447786
C                   2.957793       -1.259379       -1.725657
H                   3.085897       -0.487009       -2.494969
C                   4.246613       -1.393299       -0.951015
C                   6.682287       -1.727425        0.391054
C                   5.438304       -0.929591       -1.519279
C                   4.281069       -2.029222        0.296420
C                   5.494902       -2.189932        0.963068
C                   6.653184       -1.098079       -0.852922
H                   5.422226       -0.440495       -2.491573
H                   3.358252       -2.372011        0.758835
H                   5.512991       -2.681081        1.931932
H                   7.572631       -0.739200       -1.306151
H                   7.625953       -1.859928        0.912119
N                  -0.773340       -0.342715       -0.172512
N                   1.760423       -0.898476       -0.932853
Ru                  1.276083        0.439215        0.584973
Cl                  1.023706       -1.530186        1.963869
C                   1.613116        1.628644        2.521474
C                   2.440144        2.255999       -0.198063
C                   0.795360        2.377993        1.659988
C                   2.832000        1.108556        1.961234
C                   3.242385        1.426091        0.649933
C                   1.201166        2.681654        0.319313
H                  -0.181813        2.697366        2.000508
H                   3.428416        0.416123        2.545609
H                   4.154426        0.983885        0.263338
H                   0.540759        3.258008       -0.317083
C                   2.896937        2.648166       -1.570694
H                   2.053764        2.797602       -2.249495
H                   3.568715        1.901768       -2.000175
H                   3.452461        3.591995       -1.513684
C                   1.265907        1.310843        3.956791
H                   1.549067        0.262233        4.111414
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C	-0.217808	1.447899	4.290369
H	-0.393493	1.105015	5.313948
H	-0.836633	0.839602	3.624738
H	-0.556072	2.489618	4.239439
C	2.132827	2.189441	4.878096
H	1.953503	1.917725	5.922585
H	1.887316	3.250483	4.758954
H	3.202387	2.064851	4.680681

$\mathbf{R}_P\mathbf{SS}_M$-$[\mathbf{1}]^+$: C4

84

Enegy: -2248.37117882

C	-4.121976	-0.994451	1.291081
C	-2.397768	1.191716	0.648559
C	-2.894317	-1.257127	0.586114
C	-4.232674	0.234366	1.915970
C	-3.411812	1.324992	1.568772
C	-1.982616	-0.148668	0.349258
H	-5.106203	0.433066	2.530626
H	-3.720427	2.317799	1.888425
C	-1.993794	2.357524	-0.231866
H	-1.177102	2.030403	-0.877151
H	-1.630439	3.202984	0.363189
C	-5.406851	-1.805078	1.200473
H	-6.080421	-1.396414	1.959520
H	-5.287820	-2.860519	1.448920
C	-6.142427	-1.693806	-0.198044
H	-7.219051	-1.764345	-0.008513
H	-5.875867	-2.552628	-0.823466
C	-3.164541	2.916581	-1.146710
H	-2.708452	3.264897	-2.080998
H	-3.601972	3.796456	-0.664164
C	-4.247134	1.897750	-1.392406
C	-5.770596	-0.420850	-0.914524
C	-5.467701	1.973550	-0.710282
C	-3.965623	0.712170	-2.080152
C	-4.718299	-0.433598	-1.839274
C	-6.228116	0.827307	-0.477870
H	-5.766533	2.912065	-0.248014
H	-3.079275	0.645532	-2.708170
H	-4.406831	-1.376782	-2.282936
H	-7.105970	0.890399	0.161623
C	-2.530982	-2.534308	0.058034
C	-1.387600	-2.616304	-0.715769
H	-1.088071	-3.553761	-1.171253
C	-0.514133	-1.532117	-0.775865
C	-3.267004	-3.816266	0.330201
H	-4.246986	-3.848861	-0.153689
H	-3.415363	-3.961274	1.403883
H	-2.688944	-4.664072	-0.043202
C	0.820002	-1.679003	-1.336152
O	1.084393	-2.619635	-2.236308
C	2.524477	-2.579210	-2.437938
H	2.951973	-3.454587	-1.941898
H	2.713231	-2.624246	-3.510541
C	2.978069	-1.253195	-1.774822
H	3.107079	-0.473070	-2.536136
C	4.265956	-1.395583	-1.000503
C	6.698770	-1.741978	0.343455
C	5.458797	-0.927223	-1.562334
C	4.297681	-2.041957	0.241618
C	5.510135	-2.209122	0.909121
C	6.672332	-1.101855	-0.895068
H	5.444813	-0.430003	-2.530537
H	3.373587	-2.388112	0.698992
H	5.526296	-2.708603	1.873743
H	7.592789	-0.739322	-1.343316
H	7.641372	-1.879273	0.865210
N	-0.748838	-0.343738	-0.209530
N	1.782122	-0.898813	-0.977322
Ru	1.303450	0.418989	0.564430
Cl	1.023037	-1.575775	1.899209
C	1.607350	1.614908	2.509595
C	2.478637	2.232096	-0.200122
C	0.798073	2.344385	1.618315

C	2.836427	1.098334	1.976691
C	3.265028	1.407251	0.667069
C	1.226742	2.654884	0.288133
H	-0.188694	2.654778	1.942678
H	3.433216	0.416745	2.569943
H	4.186758	0.967907	0.300791
H	0.574867	3.223756	-0.363660
C	2.962506	2.618882	-1.564905
H	2.133840	2.752800	-2.264540
H	3.653746	1.877640	-1.971657
H	3.504803	3.569989	-1.502083
C	1.149786	1.373256	3.936935
H	0.147483	0.930043	3.871533
C	1.037325	2.725454	4.666184
H	0.666235	2.566302	5.682960
H	0.351446	3.416056	4.166089
H	2.014927	3.214274	4.740627
C	2.041163	0.415469	4.727692
H	1.613988	0.263533	5.723031
H	3.047701	0.827069	4.869271
H	2.114157	-0.561632	4.244476

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{1}]^+$: C1

84
Enegy: -2248.37998356

C	-4.307404	-0.957028	-0.900398
C	-2.313126	-0.930900	1.162545
C	-3.042524	-0.312894	-1.153908
C	-4.356282	-1.821041	0.175826
C	-3.397394	-1.779894	1.203701
C	-1.996872	-0.382283	-0.130670
H	-5.259734	-2.400082	0.345999
H	-3.628331	-2.291992	2.134976
C	-1.747282	-0.438956	2.476158
H	-0.698649	-0.160016	2.393537
H	-1.825782	-1.259148	3.198382
C	-5.654374	-0.614057	-1.523295
H	-6.340312	-1.406051	-1.209218
H	-5.662650	-0.635424	-2.613201
C	-6.265442	0.766584	-1.035936
H	-7.347140	0.628619	-0.933404
H	-6.118281	1.525679	-1.812014
C	-2.501555	0.824133	3.096757
H	-1.777818	1.643536	3.131691
H	-2.767303	0.578598	4.130052
C	-3.716386	1.240802	2.315475
C	-5.627109	1.233023	0.246853
C	-4.962421	0.626337	2.499004
C	-3.570048	2.086583	1.210281
C	-4.516648	2.082666	0.189554
C	-5.909454	0.621629	1.475127
H	-5.150650	0.049287	3.402067
H	-2.654597	2.662841	1.094489
H	-4.327648	2.657904	-0.714581
H	-6.818769	0.035457	1.591312
C	-2.755816	0.410147	-2.350399
C	-1.526825	1.035448	-2.453160
H	-1.272236	1.626742	-3.325933
C	-0.545732	0.809755	-1.490762
C	-3.668293	0.507662	-3.541422
H	-3.155909	1.014489	-4.361883
H	-4.577252	1.074193	-3.322929
H	-3.966156	-0.483137	-3.895791
C	0.823149	1.238944	-1.721342
O	1.130704	2.068372	-2.716296
C	2.551572	2.348515	-2.549241
H	3.006802	2.381861	-3.538503
H	2.641588	3.320400	-2.055239
C	3.060578	1.198071	-1.657968
N	-0.730566	0.075275	-0.385466
N	1.792564	0.763350	-1.020073
Ru	1.227407	-0.518303	0.499557
Cl	1.059744	1.495510	1.811456
C	2.037384	-2.439836	-0.408765
C	1.788464	-1.718159	2.399397

C	0.862587	-2.707899	0.330014
C	3.060530	-1.708107	0.278804
C	2.938612	-1.327837	1.632364
C	0.758958	-2.395777	1.723089
H	0.009085	-3.162545	-0.161009
H	3.935148	-1.375098	-0.272167
H	3.707432	-0.713532	2.088097
H	-0.157191	-2.638076	2.247652
C	1.689434	-1.341343	3.843147
H	1.850027	-0.265960	3.966840
H	2.463254	-1.870006	4.411243
H	0.716427	-1.600530	4.263615
C	2.248411	-2.880143	-1.841865
H	2.841904	-2.095479	-2.330796
C	0.956828	-3.060634	-2.640420
H	0.372059	-3.913833	-2.279903
H	1.195975	-3.260316	-3.688922
H	0.323791	-2.168608	-2.602825
C	3.088626	-4.170008	-1.850822
H	2.546060	-4.991767	-1.371282
H	4.039807	-4.041574	-1.324846
H	3.310719	-4.468242	-2.880031
C	4.204795	1.578161	-0.752314
C	6.405693	2.337025	0.805979
C	4.040551	2.477172	0.307798
C	5.479612	1.067517	-1.025734
C	6.577464	1.445976	-0.252729
C	5.136693	2.848268	1.084365
H	3.053902	2.859934	0.549846
H	5.621415	0.379483	-1.857672
H	7.562271	1.048308	-0.479950
H	4.997243	3.539048	1.910786
H	7.257432	2.634487	1.410744
H	3.390094	0.359874	-2.288617

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{1}]^+$: C2

84
Enegy: -2248.37712702

C	-4.204633	-0.916646	-1.189392
C	-2.274893	-1.076384	0.921451
C	-2.921139	-0.285359	-1.364376
C	-4.298782	-1.859555	-0.185154
C	-3.364323	-1.917251	0.864393
C	-1.908716	-0.428788	-0.313529
H	-5.216678	-2.431570	-0.082173
H	-3.624708	-2.498702	1.746061
C	-1.739948	-0.690502	2.283370
H	-0.807626	-0.139528	2.183777
H	-1.540767	-1.598207	2.864639
C	-5.525758	-0.484047	-1.812080
H	-6.252514	-1.256532	-1.543629
H	-5.522751	-0.449448	-2.902090
C	-6.072458	0.893809	-1.260564
H	-7.166682	0.846208	-1.287829
H	-5.774925	1.705063	-1.934080
C	-2.730618	0.206787	3.150030
H	-2.117814	0.976693	3.630839
H	-3.160887	-0.407567	3.947352
C	-3.837063	0.816226	2.332731
C	-5.542267	1.173621	0.122232
C	-5.122479	0.260372	2.326099
C	-3.543340	1.781145	1.362553
C	-4.387003	1.952035	0.268681
C	-5.972121	0.440759	1.234020
H	-5.418928	-0.416180	3.125047
H	-2.590875	2.306030	1.395720
H	-4.081588	2.613704	-0.539385
H	-6.915258	-0.100535	1.195977
C	-2.588048	0.481210	-2.519173
C	-1.347939	1.089564	-2.554241
H	-1.053102	1.709467	-3.393716
C	-0.407318	0.819444	-1.564201
C	-3.454430	0.633013	-3.739029
H	-4.352225	1.224793	-3.542023
H	-3.770442	-0.339870	-4.125495

H	-2.896374	1.140029	-4.529059
C	0.962346	1.273783	-1.731343
O	1.294387	2.103597	-2.718604
C	2.699884	2.415868	-2.497108
H	3.196333	2.439508	-3.466713
H	2.749621	3.398843	-2.019825
C	3.194919	1.293743	-1.560510
N	-0.632497	0.039724	-0.496248
N	1.910456	0.827833	-0.984562
Ru	1.311751	-0.475993	0.502873
Cl	0.902449	1.535366	1.765883
C	1.600952	-2.692883	-0.105230
C	2.570522	-1.247248	2.226133
C	0.823439	-2.577022	1.096288
C	2.829005	-1.996365	-0.114613
C	3.311711	-1.278996	1.024843
C	1.303990	-1.912910	2.242434
H	-0.169261	-3.015177	1.125528
H	3.418906	-1.973909	-1.023619
H	4.239218	-0.721558	0.953909
H	0.688714	-1.851653	3.131331
C	3.068715	-0.517055	3.431871
H	2.251669	-0.018277	3.956745
H	3.812307	0.234676	3.161832
H	3.534725	-1.237461	4.115448
C	1.136883	-3.580592	-1.249949
H	1.065100	-4.582481	-0.798201
C	2.139577	-3.676432	-2.400876
H	1.778243	-4.395143	-3.141552
H	3.124269	-4.019981	-2.068406
H	2.258898	-2.715643	-2.915445
C	-0.255876	-3.218848	-1.779226
H	-0.584095	-3.972495	-2.501133
H	-0.234843	-2.249554	-2.287231
H	-1.009091	-3.169891	-0.988672
C	4.266532	1.734216	-0.595215
C	6.329172	2.617154	1.081609
C	5.582605	1.303810	-0.801550
C	3.989424	2.612521	0.458831
C	5.017564	3.046559	1.293940
C	6.611809	1.744690	0.031017
H	5.809703	0.627669	-1.623937
H	2.968170	2.929201	0.649016
H	4.791778	3.722830	2.113386
H	7.630023	1.409446	-0.143567
H	7.127715	2.963474	1.731305
H	3.591121	0.458422	-2.155181

$\mathbf{R}_P\mathbf{RS}_M$-$[\mathbf{1}]^+$: C1

84
Enegy: -2248.36991737

C	-4.204545	-1.410919	-0.249642
C	-2.218275	-0.478765	1.579688
C	-3.029368	-0.759105	-0.765678
C	-4.153620	-1.847789	1.062060
C	-3.203475	-1.354326	1.975956
C	-1.982490	-0.378890	0.169447
H	-4.989232	-2.418966	1.457032
H	-3.375219	-1.524611	3.036376
C	-1.660172	0.541006	2.546514
H	-0.765466	0.988632	2.111894
H	-1.374485	0.053951	3.485243
C	-5.581718	-1.434700	-0.897669
H	-6.186298	-2.126157	-0.303587
H	-5.588420	-1.834806	-1.912347
C	-6.323931	-0.033097	-0.900057
H	-7.391652	-0.226754	-0.750968
H	-6.224176	0.433654	-1.885846
C	-2.670466	1.714242	2.938768
H	-2.115947	2.657661	2.885115
H	-2.963584	1.578956	3.984534
C	-3.899187	1.759805	2.071821
C	-5.762214	0.891386	0.149304
C	-5.078766	1.113616	2.463064
C	-3.822510	2.220721	0.753142

C	-4.745351	1.790198	-0.195970
C	-6.004800	0.685898	1.512516
H	-5.218282	0.834975	3.505463
H	-2.971110	2.820591	0.437525
H	-4.599279	2.058814	-1.239923
H	-6.849655	0.076796	1.826756
C	-2.845243	-0.404310	-2.138537
C	-1.740717	0.358095	-2.468664
H	-1.576050	0.689221	-3.488011
C	-0.727385	0.551013	-1.529816
C	-3.734670	-0.846260	-3.266559
H	-4.720848	-0.375193	-3.234114
H	-3.877343	-1.930340	-3.248939
H	-3.278461	-0.586483	-4.224034
C	0.571749	1.061759	-1.936474
O	0.726160	1.714930	-3.080934
C	2.139983	2.041631	-3.175931
H	2.498926	1.683233	-4.141410
H	2.230555	3.128906	-3.122940
C	2.798341	1.327617	-1.961966
N	-0.787315	0.133269	-0.260670
N	1.621621	0.839904	-1.220442
Ru	1.358984	-0.585388	0.272784
Cl	0.856999	-2.054093	-1.571856
C	2.663070	-2.330450	1.002496
C	2.065095	0.172341	2.351281
C	1.509425	-2.198844	1.830959
C	3.434214	-1.163073	0.770008
C	3.134587	0.064467	1.433286
C	1.225420	-0.975391	2.476971
H	0.830063	-3.036590	1.943022
H	4.257669	-1.195901	0.067280
H	3.738770	0.939396	1.216366
H	0.333931	-0.911922	3.086926
C	1.864045	1.420183	3.157658
H	0.828734	1.544121	3.478222
H	2.170681	2.307987	2.599345
H	2.483108	1.367143	4.061572
C	3.000671	-3.675398	0.401295
H	2.057315	-4.096686	0.034007
C	3.532617	-4.580152	1.531201
H	3.729808	-5.580304	1.134238
H	2.817546	-4.681742	2.353316
H	4.470716	-4.191519	1.942233
C	3.983329	-3.624007	-0.766756
H	4.101675	-4.627779	-1.184485
H	4.978416	-3.289930	-0.449882
H	3.617063	-2.974516	-1.566274
H	3.358016	0.445350	-2.294841
C	3.715562	2.225605	-1.163812
C	5.442030	3.926303	0.246369
C	5.097606	2.017823	-1.195690
C	3.204035	3.297734	-0.421365
C	4.062035	4.142252	0.280370
C	5.958748	2.864629	-0.494743
H	5.506862	1.193996	-1.776857
H	2.130616	3.470339	-0.388397
H	3.656285	4.973903	0.849604
H	7.030937	2.695425	-0.531556
H	6.110045	4.587811	0.789948

$\mathbf{R}_P\mathbf{RS}_M$-$[\mathbf{1}]^+$: C2

84
Enegy: -2248.36991624

C	-4.212753	-1.424158	-0.221702
C	-2.224491	-0.472825	1.595522
C	-3.038354	-0.777427	-0.745843
C	-4.160065	-1.847661	1.094285
C	-3.208877	-1.344660	2.001864
C	-1.990430	-0.387138	0.184033
H	-4.995024	-2.414960	1.496161
H	-3.379177	-1.504269	3.064175
C	-1.665584	0.556714	2.551462
H	-0.772029	1.000847	2.110991
H	-1.377868	0.078978	3.494352

C	-5.590769	-1.454648	-0.867677
H	-6.194583	-2.139867	-0.265645
H	-5.598815	-1.865269	-1.878134
C	-6.332907	-0.053131	-0.883657
H	-7.400520	-0.245207	-0.731766
H	-6.233925	0.403652	-1.874181
C	-2.676161	1.732802	2.934158
H	-2.122229	2.676017	2.871507
H	-2.968256	1.606789	3.981368
C	-3.905714	1.769712	2.067974
C	-5.770298	0.881875	0.155876
C	-5.084833	1.127245	2.466698
C	-3.830244	2.217398	0.744694
C	-4.753811	1.777229	-0.199276
C	-6.011659	0.689985	1.521293
H	-5.223349	0.858973	3.511945
H	-2.979183	2.814164	0.422346
H	-4.608606	2.035302	-1.246003
H	-6.856175	0.083960	1.842323
C	-2.855978	-0.437193	-2.122580
C	-1.751989	0.321851	-2.462062
H	-1.588511	0.642062	-3.485078
C	-0.737742	0.525252	-1.526435
C	-3.746585	-0.891320	-3.244822
H	-4.732788	-0.420047	-3.216350
H	-3.889093	-1.975167	-3.215440
H	-3.291452	-0.641748	-4.205518
C	0.560586	1.032143	-1.940344
O	0.713146	1.672466	-3.092315
C	2.126600	1.999041	-3.192685
H	2.484411	1.631159	-4.155006
H	2.216577	3.086864	-3.150790
C	2.787071	1.297798	-1.972527
N	-0.796030	0.121140	-0.252798
N	1.611575	0.818685	-1.223418
Ru	1.352166	-0.589745	0.286255
Cl	0.848700	-2.079626	-1.540945
C	2.660504	-2.324160	1.032656
C	2.059225	0.191535	2.355735
C	1.507696	-2.186133	1.861354
C	3.429082	-1.157815	0.787048
C	3.127856	0.076082	1.437712
C	1.222126	-0.956582	2.494866
H	0.830128	-3.023987	1.983060
H	4.251757	-1.196329	0.083694
H	3.730155	0.949807	1.210946
H	0.331347	-0.888476	3.105362
C	1.856552	1.447728	3.148640
H	2.480271	1.407980	4.050020
H	0.822272	1.570789	3.472806
H	2.156449	2.330304	2.578486
C	3.000007	-3.674645	0.445113
H	2.056938	-4.101901	0.084046
C	3.536013	-4.566198	1.583554
H	3.734657	-5.570077	1.196850
H	2.822671	-4.660620	2.408023
H	4.474012	-4.171193	1.988695
C	3.980412	-3.633480	-0.725241
H	3.611273	-2.993251	-1.530884
H	4.100147	-4.641342	-1.132597
H	4.975362	-3.293971	-0.413763
H	3.345433	0.411543	-2.296969
C	3.706429	2.203822	-1.186047
C	5.436661	3.918300	0.202708
C	5.088212	1.994308	-1.217619
C	3.197084	3.284717	-0.454878
C	4.056937	4.136073	0.236239
C	5.951224	2.847953	-0.527343
H	5.495806	1.163693	-1.790227
H	2.123892	3.458807	-0.422292
H	3.652849	4.974396	0.796797
H	7.023187	2.677254	-0.563819
H	6.106130	4.585082	0.737991

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C1

83

Enegy: -2135.31666724

C	-3.812126	0.274586	-1.528930
C	-1.931299	-1.488935	-0.270397
C	-2.548568	0.802036	-1.077142
C	-3.897574	-1.097094	-1.657282
C	-2.990620	-1.959298	-1.015487
C	-1.563777	-0.115223	-0.498517
H	-4.796137	-1.531955	-2.086315
H	-3.252081	-3.012808	-0.948202
C	-1.445068	-2.341099	0.879335
H	-0.393326	-2.174524	1.104616
H	-1.565127	-3.389444	0.584668
C	-5.131492	1.027169	-1.637966
H	-5.826185	0.344997	-2.136526
H	-5.091929	1.916292	-2.267640
C	-5.769529	1.422330	-0.241068
H	-6.855614	1.316210	-0.335794
H	-5.574109	2.480730	-0.036730
C	-2.238499	-2.125821	2.247665
H	-1.525237	-1.723235	2.972569
H	-2.550795	-3.110826	2.609312
C	-3.417576	-1.202181	2.114252
C	-5.210329	0.586968	0.881783
C	-4.660328	-1.648859	1.644951
C	-3.227050	0.180080	2.219725
C	-4.114538	1.063091	1.610502
C	-5.548808	-0.763856	1.034680
H	-4.887496	-2.712941	1.650840
H	-2.318195	0.561603	2.680080
H	-3.885987	2.126970	1.601821
H	-6.452347	-1.151290	0.568338
C	-2.208157	2.184857	-1.156566
C	-0.991065	2.584953	-0.636414
H	-0.695081	3.628267	-0.646477
C	-0.074487	1.637127	-0.189356
C	-3.047132	3.243955	-1.816189
H	-3.317558	2.959471	-2.836783
H	-2.489351	4.181440	-1.867638
H	-3.971022	3.443061	-1.266298
C	1.279752	2.029698	0.166546
O	1.616357	3.309547	0.294802
C	3.066357	3.323073	0.450492
H	3.484054	3.720263	-0.478458
H	3.300703	3.995744	1.275301
C	3.449536	1.846513	0.714468
N	-0.307440	0.316911	-0.162917
N	2.204527	1.151102	0.327252
Ru	1.629068	-0.803310	-0.064844
Cl	1.394464	-0.985732	2.320465
C	2.595831	-0.950811	-2.120879
C	2.067944	-3.071749	-0.197589
C	1.375001	-1.660007	-2.108694
C	3.522044	-1.269795	-1.072086
C	3.265410	-2.279582	-0.121456
C	1.131009	-2.729278	-1.186575
H	0.589318	-1.392081	-2.806516
H	4.430324	-0.681802	-0.976491
H	3.964174	-2.445964	0.691288
H	0.177831	-3.243815	-1.221781
C	1.829088	-4.160456	0.799209
H	1.913177	-3.767401	1.817498
H	2.584716	-4.943877	0.672498
H	0.842944	-4.611170	0.677276
C	2.953824	0.098974	-3.150955
H	3.510842	0.884404	-2.621338
C	1.747596	0.749980	-3.828245
H	2.082123	1.572269	-4.467211
H	1.037948	1.156314	-3.100712
H	1.213906	0.043131	-4.472859
C	3.902378	-0.522695	-4.192002
H	3.399203	-1.318649	-4.751228
H	4.796542	-0.950272	-3.727732
H	4.227175	0.238660	-4.907692
H	4.243566	1.535393	0.026454
C	3.908738	1.530356	2.152813
H	3.910372	0.436267	2.231662
C	5.339505	2.039225	2.356721
H	5.401161	3.131645	2.276463
H	6.037153	1.609578	1.628604
H	5.697323	1.772069	3.355179
C	2.963131	2.067429	3.228050

H	1.937865	1.721729	3.075244
H	2.970356	3.162655	3.277499
H	3.279381	1.702534	4.209567

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C2

83
Enegy: -2135.31451271

C	-3.840442	0.432866	-1.425986
C	-1.978717	-1.366804	-0.202448
C	-2.536717	0.921024	-1.047405
C	-3.977925	-0.932867	-1.543186
C	-3.072550	-1.811255	-0.918289
C	-1.571067	-0.011468	-0.457515
H	-4.908534	-1.343906	-1.925827
H	-3.358274	-2.856903	-0.836390
C	-1.501246	-2.227003	0.947454
H	-0.423693	-2.181125	1.100397
H	-1.765724	-3.262414	0.704369
C	-5.109902	1.276387	-1.455060
H	-5.579223	1.241617	-2.446112
H	-4.873225	2.318641	-1.262074
C	-6.182149	0.841842	-0.378742
H	-6.877805	0.119433	-0.817518
H	-6.771695	1.732405	-0.130407
C	-2.159555	-1.865549	2.343547
H	-1.455630	-1.228776	2.886688
H	-2.253745	-2.799102	2.908971
C	-3.479076	-1.160755	2.188225
C	-5.519723	0.225120	0.829044
C	-4.637641	-1.830144	1.780538
C	-3.504669	0.240403	2.171296
C	-4.519126	0.926993	1.511781
C	-5.642762	-1.142827	1.096516
H	-4.698979	-2.912789	1.871089
H	-2.663293	0.793347	2.583611
H	-4.452651	2.008903	1.414709
H	-6.465732	-1.703085	0.657250
C	-2.127295	2.271475	-1.244959
C	-0.893452	2.653702	-0.746554
H	-0.547821	3.678041	-0.837657
C	-0.019656	1.699393	-0.235433
C	-2.888147	3.306139	-2.033478
H	-3.579174	3.877219	-1.403232
H	-3.459974	2.865319	-2.851513
H	-2.185851	4.026045	-2.461942
C	1.346884	2.058349	0.110711
O	1.721787	3.330034	0.210306
C	3.170925	3.303311	0.372612
H	3.604575	3.668695	-0.562065
H	3.421620	3.985659	1.184599
C	3.508625	1.821778	0.669478
N	-0.297531	0.388827	-0.153941
N	2.244232	1.155938	0.293233
Ru	1.611097	-0.787186	-0.075321
Cl	1.419643	-0.957153	2.312319
C	2.539752	-0.969020	-2.147447
C	1.980017	-3.067710	-0.208976
C	1.298734	-1.640986	-2.113603
C	3.471953	-1.310753	-1.110953
C	3.201058	-2.310614	-0.153693
C	1.037180	-2.698758	-1.182773
H	0.510715	-1.352331	-2.800410
H	4.398049	-0.748796	-1.030814
H	3.907022	-2.494900	0.648932
H	0.067602	-3.183184	-1.199424
C	1.724958	-4.146787	0.794348
H	0.723970	-4.568307	0.689202
H	1.837381	-3.754278	1.810178
H	2.454728	-4.952671	0.657372
C	2.913884	0.066033	-3.186695
H	3.494518	0.840592	-2.666437
C	1.718047	0.742301	-3.857498
H	2.067031	1.551830	-4.505005
H	1.025220	1.170837	-3.126489
H	1.161339	0.044500	-4.492458

C	3.837873	-0.583998	-4.232507
H	3.310658	-1.370389	-4.783044
H	4.725444	-1.030764	-3.773719
H	4.174809	0.165485	-4.955100
H	4.295183	1.472042	-0.008519
C	3.953549	1.523685	2.116014
H	3.931139	0.431641	2.215853
C	5.393890	2.005395	2.318261
H	5.479892	3.094678	2.219698
H	6.085400	1.548068	1.601224
H	5.741157	1.747697	3.322915
C	3.013290	2.101255	3.174730
H	1.982887	1.769704	3.024706
H	3.038931	3.197098	3.199684
H	3.318967	1.753010	4.165611

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C1

83
Enegy: -2135.31667999

C	-3.969685	0.089873	-1.275858
C	-1.988941	-1.485844	0.074823
C	-2.681796	0.673134	-0.992381
C	-4.051850	-1.286401	-1.208547
C	-3.094317	-2.053205	-0.520608
C	-1.650442	-0.157308	-0.366044
H	-4.974714	-1.775115	-1.508685
H	-3.341273	-3.087064	-0.290601
C	-1.413009	-2.172012	1.292097
H	-0.348776	-1.978442	1.413592
H	-1.546137	-3.250726	1.154535
C	-5.300317	0.821404	-1.391543
H	-6.022331	0.078003	-1.741581
H	-5.313806	1.616454	-2.137414
C	-5.841145	1.403477	-0.019121
H	-6.929976	1.284102	-0.019598
H	-5.643464	2.480174	0.024011
C	-2.105604	-1.767650	2.672244
H	-1.345091	-1.268223	3.279260
H	-2.380642	-2.692513	3.189482
C	-3.300309	-0.871075	2.499061
C	-5.194148	0.730568	1.164079
C	-4.568928	-1.378290	2.186610
C	-3.116602	0.512534	2.399104
C	-4.054108	1.302877	1.739436
C	-5.507431	-0.586157	1.525730
H	-4.784536	-2.431339	2.355500
H	-2.181095	0.954068	2.735823
H	-3.837412	2.355378	1.567930
H	-6.438085	-1.034291	1.183651
C	-2.359771	2.031627	-1.284181
C	-1.111474	2.497175	-0.913983
H	-0.825741	3.528787	-1.088184
C	-0.156963	1.618001	-0.409629
C	-3.253952	2.991952	-2.018103
H	-3.594352	2.572136	-2.968662
H	-2.710532	3.913895	-2.235689
H	-4.137772	3.263305	-1.434361
C	1.216613	2.052670	-0.212030
O	1.552153	3.337130	-0.285824
C	3.009633	3.367707	-0.242727
H	3.353623	3.630989	-1.246492
H	3.300042	4.147442	0.461116
C	3.422347	1.940697	0.193119
N	-0.376708	0.314413	-0.185136
N	2.157500	1.202110	-0.001672
Ru	1.570845	-0.786202	-0.077523
Cl	1.515766	-0.639669	2.321190
C	2.386580	-1.215352	-2.159210
C	2.015483	-3.052589	0.068593
C	3.389045	-1.390959	-1.147285
C	1.175332	-1.913421	-1.961798
C	1.006945	-2.846217	-0.887134
C	3.209570	-2.260750	-0.051714
H	4.297662	-0.798026	-1.199252
H	0.339072	-1.741388	-2.630409

H	0.057560	-3.358283	-0.782437
H	3.966607	-2.316179	0.723101
C	1.857421	-3.994062	1.219508
H	0.867624	-4.452986	1.233508
H	2.014143	-3.466047	2.165619
H	2.606207	-4.790681	1.145263
C	2.661417	-0.315957	-3.345401
H	3.243063	0.536447	-2.967415
C	1.404561	0.232215	-4.021655
H	1.685482	0.958977	-4.789270
H	0.740601	0.733720	-3.310572
H	0.837112	-0.558415	-4.524539
C	3.545382	-1.071757	-4.354080
H	3.015481	-1.938194	-4.763884
H	4.473849	-1.429225	-3.897949
H	3.812149	-0.414685	-5.187422
H	4.166018	1.535572	-0.502229
C	3.987782	1.823792	1.623530
H	4.002741	0.750812	1.851072
C	5.425927	2.351558	1.650482
H	6.071756	1.823788	0.939267
H	5.857412	2.223169	2.647311
H	5.473696	3.422359	1.416586
C	3.119136	2.506196	2.681130
H	3.508164	2.278251	3.677739
H	2.087827	2.146137	2.652074
H	3.122554	3.597828	2.579377

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C2

83
Enegy: -2135.31668496

C	-4.017939	0.043886	-1.200595
C	-2.016488	-1.501152	0.155171
C	-2.726075	0.633274	-0.949803
C	-4.098709	-1.330511	-1.100985
C	-3.130639	-2.081658	-0.410576
C	-1.685106	-0.182911	-0.320638
H	-5.025882	-1.825816	-1.375984
H	-3.373817	-3.110064	-0.153663
C	-1.422413	-2.159970	1.378824
H	-0.356043	-1.966139	1.479249
H	-1.559750	-3.241266	1.268377
C	-5.350352	0.772720	-1.312515
H	-6.077422	0.021709	-1.634747
H	-5.375324	1.550775	-2.075810
C	-5.870415	1.385628	0.054501
H	-6.959050	1.265989	0.073447
H	-5.672729	2.463069	0.070116
C	-2.092244	-1.722239	2.759984
H	-1.322041	-1.208157	3.342034
H	-2.358110	-2.634376	3.303935
C	-3.290056	-0.830193	2.584883
C	-5.204965	0.740023	1.242634
C	-4.562957	-1.344793	2.303402
C	-3.108885	0.550863	2.450790
C	-4.056815	1.325690	1.787593
C	-5.511870	-0.568227	1.638949
H	-4.775248	-2.393791	2.499484
H	-2.168750	1.000290	2.763295
H	-3.843511	2.374130	1.589059
H	-6.447330	-1.024303	1.321361
C	-2.408889	1.984911	-1.276768
C	-1.155377	2.458678	-0.935827
H	-0.872667	3.486138	-1.137350
C	-0.193015	1.590970	-0.426564
C	-3.314273	2.928465	-2.018651
H	-4.189608	3.212502	-1.428225
H	-3.668293	2.487512	-2.954559
H	-2.774623	3.845475	-2.264634
C	1.183354	2.029740	-0.259704
O	1.517420	3.312225	-0.366982
C	2.975357	3.343570	-0.347131
H	3.303736	3.584598	-1.361658
H	3.276468	4.138591	0.334760
C	3.395063	1.926475	0.113721

N	-0.408892	0.292727	-0.169876
N	2.127545	1.183899	-0.045115
Ru	1.540076	-0.805645	-0.069936
Cl	1.524055	-0.608989	2.325628
C	2.321815	-1.279106	-2.155304
C	1.987130	-3.068341	0.116999
C	3.340512	-1.433198	-1.156087
C	1.114018	-1.972390	-1.923263
C	0.963038	-2.881796	-0.826213
C	3.179086	-2.279641	-0.039576
H	4.247992	-0.841506	-1.235185
H	0.267025	-1.814483	-2.581786
H	0.015458	-3.391134	-0.695155
H	3.948590	-2.318656	0.723870
C	1.847801	-3.985073	1.290087
H	0.858369	-4.443274	1.329866
H	2.019803	-3.437099	2.222098
H	2.595328	-4.783300	1.220659
C	2.577443	-0.405952	-3.365140
H	3.164394	0.454775	-3.015288
C	1.309783	0.126622	-4.033685
H	0.735082	-0.675219	-4.509880
H	1.578196	0.836161	-4.821616
H	0.656629	0.643691	-3.323738
C	3.445963	-1.183686	-4.370573
H	2.910267	-2.059234	-4.752537
H	4.381771	-1.530566	-3.921330
H	3.699056	-0.545248	-5.222454
H	4.128019	1.505955	-0.583863
C	3.982588	1.841423	1.537453
H	4.002254	0.773742	1.788324
C	5.420422	2.370670	1.530565
H	5.463548	3.436159	1.272715
H	6.055684	1.827947	0.821093
H	5.867421	2.264324	2.523143
C	3.129569	2.546261	2.593046
H	3.533867	2.340248	3.588349
H	2.098239	2.185136	2.587468
H	3.130524	3.635426	2.467549

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C3

83
Enegy: -2135.31787435

C	-3.715331	0.383069	-1.587925
C	-1.855424	-1.357657	-0.275364
C	-2.448754	0.913704	-1.150958
C	-3.811767	-0.991078	-1.680333
C	-2.911318	-1.842351	-1.015511
C	-1.473450	0.008341	-0.535859
H	-4.713196	-1.430118	-2.098710
H	-3.179126	-2.892351	-0.920872
C	-1.374638	-2.175496	0.903658
H	-0.443303	-1.775060	1.296949
H	-1.187396	-3.205563	0.577791
C	-5.028632	1.144505	-1.708390
H	-5.738841	0.450576	-2.167746
H	-4.992416	2.009717	-2.371162
C	-5.635060	1.594150	-0.318236
H	-6.725884	1.587878	-0.420050
H	-5.343810	2.628977	-0.106856
C	-2.405349	-2.248996	2.117357
H	-1.821693	-2.112100	3.033700
H	-2.836013	-3.254542	2.155738
C	-3.508287	-1.230792	2.012586
C	-5.155911	0.703405	0.799449
C	-4.771874	-1.578261	1.518340
C	-3.221084	0.131738	2.153206
C	-4.035243	1.085064	1.547987
C	-5.592724	-0.620497	0.921554
H	-5.068822	-2.624687	1.491945
H	-2.291755	0.439656	2.627846
H	-3.730030	2.129492	1.559819
H	-6.514363	-0.935018	0.436136
C	-2.099177	2.289394	-1.285219
C	-0.881530	2.700307	-0.776895

H	-0.575200	3.739227	-0.830351
C	0.023528	1.765869	-0.282477
C	-2.924183	3.325879	-1.996892
H	-2.352643	4.251239	-2.095394
H	-3.844463	3.566705	-1.457816
H	-3.199671	2.994481	-3.001804
C	1.374155	2.173579	0.069543
O	1.723201	3.456743	0.099493
C	3.170944	3.469022	0.277283
H	3.606721	3.792843	-0.671473
H	3.399067	4.198598	1.054105
C	3.535722	2.012299	0.655175
N	-0.216645	0.447694	-0.202826
N	2.286640	1.303429	0.315151
Ru	1.700443	-0.668209	0.070719
Cl	1.302288	-0.610806	2.444201
C	1.790247	-1.488267	-2.059623
C	3.110002	-2.417463	0.353935
C	3.052997	-0.991997	-1.676972
C	1.178108	-2.450878	-1.184043
C	1.811982	-2.909157	-0.018781
C	3.702553	-1.450131	-0.484393
H	3.525319	-0.212516	-2.264394
H	0.172178	-2.789517	-1.409611
H	1.296167	-3.592402	0.646562
H	4.654818	-1.016765	-0.196033
C	3.773399	-2.898814	1.604977
H	3.079239	-2.861210	2.448725
H	4.649679	-2.296208	1.851932
H	4.098343	-3.936741	1.467409
C	1.075108	-1.080116	-3.329488
H	0.006946	-1.023661	-3.080986
C	1.252849	-2.189137	-4.382790
H	0.682344	-1.944987	-5.283980
H	0.903451	-3.160110	-4.018259
H	2.305335	-2.293719	-4.667457
C	1.505669	0.277187	-3.885454
H	0.865803	0.549399	-4.729596
H	2.534914	0.257151	-4.260659
H	1.423948	1.070259	-3.135423
H	4.329514	1.638892	-0.001943
C	3.978174	1.797931	2.117356
H	3.958576	0.712390	2.276578
C	5.416083	2.295126	2.297548
H	6.112304	1.802669	1.608870
H	5.761088	2.096285	3.316295
H	5.496841	3.377517	2.138149
C	3.033455	2.429399	3.140873
H	3.334467	2.132644	4.149807
H	2.003358	2.091935	3.003230
H	3.061226	3.524929	3.109539

$\mathbf{R}_P\mathbf{RR}_M$-$[\mathbf{2}]^+$: C4

83
Enegy: -2135.31336582

C	-3.781780	0.290732	-1.523780
C	-1.886474	-1.424181	-0.228981
C	-2.501660	0.827569	-1.136698
C	-3.883519	-1.084859	-1.582659
C	-2.965161	-1.922754	-0.925794
C	-1.508688	-0.066225	-0.531958
H	-4.797453	-1.531079	-1.964695
H	-3.231086	-2.969915	-0.800009
C	-1.374456	-2.217663	0.952853
H	-0.431932	-1.810947	1.311105
H	-1.200311	-3.254337	0.641676
C	-5.096919	1.052309	-1.622927
H	-5.821218	0.349536	-2.045348
H	-5.078948	1.902064	-2.306109
C	-5.661836	1.534499	-0.226394
H	-6.755162	1.529713	-0.296575
H	-5.361597	2.572639	-0.046222
C	-2.371091	-2.263874	2.196241
H	-1.761904	-2.109677	3.093027
H	-2.802427	-3.267377	2.267186

C	-3.474565	-1.245358	2.101864
C	-5.152758	0.666757	0.896082
C	-4.752788	-1.599969	1.652416
C	-3.180202	0.119031	2.204469
C	-4.009779	1.061320	1.603042
C	-5.588728	-0.652937	1.059367
H	-5.052533	-2.645925	1.657125
H	-2.236423	0.434403	2.644441
H	-3.702158	2.104926	1.583368
H	-6.524770	-0.975264	0.607820
C	-2.155000	2.199393	-1.311374
C	-0.921332	2.618172	-0.850703
H	-0.614764	3.654786	-0.936875
C	-0.001582	1.692355	-0.367044
C	-3.000274	3.222453	-2.018663
H	-2.430758	4.144424	-2.153774
H	-3.903200	3.476081	-1.456646
H	-3.306824	2.870901	-3.007584
C	1.361185	2.106639	-0.076821
O	1.714025	3.389161	-0.098423
C	3.167596	3.400817	0.020429
H	3.565857	3.686178	-0.956815
H	3.429808	4.158045	0.759067
C	3.541337	1.957408	0.437535
N	-0.240054	0.376513	-0.251082
N	2.280408	1.241958	0.161218
Ru	1.686471	-0.735263	0.009515
Cl	1.321021	-0.564124	2.380693
C	1.885151	-1.595816	-2.124420
C	2.993615	-2.555596	0.388652
C	3.132514	-1.144591	-1.638328
C	1.163708	-2.496127	-1.270940
C	1.703043	-2.982530	-0.064285
C	3.684364	-1.615533	-0.405465
H	3.687568	-0.405111	-2.207388
H	0.158337	-2.792437	-1.546297
H	1.118313	-3.646524	0.560879
H	4.635767	-1.225356	-0.059500
C	3.556404	-3.067014	1.676031
H	3.885492	-4.103674	1.536834
H	2.802484	-3.044454	2.466501
H	4.413713	-2.475646	2.002806
C	1.391833	-1.175267	-3.502691
H	2.164656	-1.545559	-4.193235
C	1.317615	0.347424	-3.674411
H	1.084115	0.593700	-4.714466
H	2.259443	0.845265	-3.425390
H	0.530272	0.768471	-3.042047
C	0.071765	-1.830997	-3.911284
H	-0.173892	-1.546460	-4.938282
H	-0.758527	-1.508284	-3.273796
H	0.127627	-2.923901	-3.883287
H	4.314071	1.558536	-0.229708
C	4.027919	1.793433	1.892516
H	4.005019	0.714815	2.093207
C	5.474643	2.284137	2.009074
H	6.145189	1.759851	1.318404
H	5.849893	2.121213	3.023502
H	5.558496	3.358923	1.805876
C	3.121523	2.471147	2.921208
H	3.450639	2.206963	3.930433
H	2.084177	2.141071	2.827338
H	3.159630	3.564441	2.849996

$\mathbf{R}_P\mathbf{R}_M$-[**3**]$^+$: C1

80
Enegy: -2096.01737295

C	-3.718894	0.041559	-1.342596
C	-1.692086	-1.447432	0.029711
C	-2.481966	0.695390	-0.998994
C	-3.719474	-1.339475	-1.315255
C	-2.739060	-2.066787	-0.617430
C	-1.421481	-0.087849	-0.361781
H	-4.601744	-1.873136	-1.657531
H	-2.929840	-3.119323	-0.420010

C	-1.104494	-2.112861	1.256214
H	-0.198343	-1.600302	1.572741
H	-0.838276	-3.149328	1.017319
C	-5.087470	0.696763	-1.471634
H	-5.759815	-0.079346	-1.849116
H	-5.134696	1.506635	-2.200471
C	-5.681040	1.213217	-0.098512
H	-6.770664	1.115041	-0.156091
H	-5.466362	2.281340	0.016643
C	-2.086231	-2.162907	2.510320
H	-1.484934	-1.912554	3.390637
H	-2.439640	-3.190324	2.642919
C	-3.265601	-1.238929	2.369043
C	-5.096688	0.458968	1.068443
C	-4.515950	-1.718273	1.958562
C	-3.078085	0.147951	2.384574
C	-3.983197	0.983993	1.736755
C	-5.427323	-0.877689	1.318319
H	-4.733415	-2.781877	2.031678
H	-2.159096	0.562764	2.793515
H	-3.758444	2.045161	1.650261
H	-6.338809	-1.298946	0.899166
C	-2.245322	2.083167	-1.230630
C	-1.059514	2.622794	-0.769217
H	-0.847248	3.681016	-0.875991
C	-0.065158	1.791848	-0.260398
C	-3.164132	3.001946	-1.987511
H	-4.086937	3.211775	-1.439845
H	-3.437754	2.579418	-2.958136
H	-2.667469	3.957793	-2.167329
C	1.250153	2.325055	0.056328
O	1.431432	3.635384	0.202774
C	2.780037	3.777804	0.727049
H	3.250158	4.615804	0.210618
H	2.689257	3.995931	1.795215
C	3.464402	2.412177	0.456785
N	-0.189146	0.465731	-0.116054
N	2.269784	1.556578	0.198453
Ru	1.813777	-0.478383	0.096573
Cl	1.567625	-0.220744	2.481025
C	1.805349	-1.476458	-1.959256
C	3.333972	-2.132438	0.421587
C	1.305664	-2.384191	-0.964113
C	3.063762	-0.892641	-1.711247
C	3.819018	-1.222188	-0.539131
C	2.037760	-2.706187	0.190003
H	0.305695	-2.786484	-1.087272
H	3.454670	-0.148707	-2.395579
H	4.772523	-0.735466	-0.364968
H	1.603013	-3.349537	0.946542
C	4.105013	-2.475287	1.656476
H	4.979042	-1.832318	1.776934
H	4.449637	-3.513984	1.593583
H	3.475074	-2.372047	2.544198
C	0.985862	-1.212354	-3.203830
H	-0.065304	-1.195125	-2.886673
C	1.161682	-2.390928	-4.178822
H	0.519809	-2.252320	-5.054052
H	0.896612	-3.347203	-3.717186
H	2.197741	-2.459508	-4.527545
C	1.296414	0.118351	-3.889080
H	0.586329	0.288181	-4.703380
H	2.297547	0.125078	-4.334221
H	1.218746	0.961460	-3.195393
C	4.332872	2.475596	-0.803767
H	5.166309	3.166861	-0.643225
H	4.758575	1.498034	-1.041008
H	3.758798	2.825930	-1.667427
C	4.261635	1.938300	1.665999
H	3.619218	1.823606	2.541121
H	5.052905	2.661730	1.888978
H	4.735051	0.973414	1.469444

$\mathbf{R}_P\mathbf{R}_M$-$[\mathbf{3}]^+$: C2

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Enegy: -2096.01448661

C	-3.778854	0.078046	-1.272454
C	-1.740533	-1.421652	0.072125
C	-2.527090	0.720002	-0.960181
C	-3.793717	-1.302148	-1.233631
C	-2.806522	-2.033695	-0.550437
C	-1.462250	-0.068117	-0.334290
H	-4.687715	-1.829434	-1.554835
H	-3.002011	-3.083516	-0.343676
C	-1.140319	-2.095425	1.285478
H	-0.184641	-1.647786	1.547895
H	-0.970001	-3.152947	1.053166
C	-5.142264	0.747377	-1.384115
H	-5.829311	-0.025673	-1.740786
H	-5.193912	1.549107	-2.121525
C	-5.705942	1.286220	-0.006875
H	-6.796538	1.187247	-0.038581
H	-5.489137	2.356118	0.085839
C	-2.055562	-2.043214	2.592533
H	-1.408900	-1.727258	3.417394
H	-2.398546	-3.057465	2.819602
C	-3.237776	-1.124392	2.450276
C	-5.095702	0.551498	1.159259
C	-4.496895	-1.610482	2.075471
C	-3.049122	0.262255	2.435333
C	-3.967914	1.087695	1.793223
C	-5.420873	-0.780757	1.439500
H	-4.714054	-2.672041	2.174516
H	-2.121208	0.682789	2.817241
H	-3.744853	2.147002	1.682775
H	-6.341652	-1.208326	1.047939
C	-2.276604	2.099379	-1.222578
C	-1.071570	2.628768	-0.801378
H	-0.846534	3.681516	-0.932561
C	-0.078714	1.793271	-0.297699
C	-3.200806	3.018998	-1.971687
H	-3.502034	2.586328	-2.929574
H	-2.696180	3.965540	-2.176781
H	-4.107886	3.248543	-1.405927
C	1.242905	2.322194	0.001139
O	1.427531	3.634554	0.117963
C	2.784518	3.795681	0.610409
H	3.259756	4.580302	0.019413
H	2.713349	4.106384	1.656488
C	3.451623	2.400817	0.446952
N	-0.217185	0.471996	-0.125011
N	2.257073	1.552030	0.167191
Ru	1.788987	-0.485524	0.073014
Cl	1.540096	-0.212048	2.452556
C	1.978108	-1.380087	-2.045379
C	3.141643	-2.275389	0.463117
C	1.284802	-2.275402	-1.169572
C	3.220808	-0.893817	-1.582400
C	3.805170	-1.335091	-0.355143
C	1.853902	-2.732394	0.038100
H	0.277815	-2.590069	-1.421320
H	3.738611	-0.145661	-2.174279
H	4.756714	-0.927483	-0.032059
H	1.293627	-3.400055	0.680647
C	3.733440	-2.755982	1.749396
H	4.116304	-3.773889	1.608260
H	2.982854	-2.773488	2.542714
H	4.558686	-2.120143	2.074704
C	1.484436	-0.991412	-3.425008
H	1.770990	0.057626	-3.579976
C	-0.026795	-1.106839	-3.619988
H	-0.298277	-0.722842	-4.607564
H	-0.584615	-0.536815	-2.873138
H	-0.363315	-2.148563	-3.580030
C	2.231500	-1.840590	-4.470900
H	1.931217	-1.541658	-5.479884
H	1.996450	-2.903947	-4.352102
H	3.316865	-1.724102	-4.393829
C	4.402376	2.385835	-0.753435
H	3.884808	2.657461	-1.679000
H	5.210629	3.105802	-0.590165
H	4.863915	1.403940	-0.880435
C	4.166492	1.975582	1.725221
H	4.975231	2.681489	1.942181
H	4.605183	0.981072	1.616990
H	3.477885	1.944140	2.571433

$\mathbf{R}_P\mathbf{R}_M$-$[\mathbf{3}]^+$: C3

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80
Enegy:  -2096.01278582
C                -3.711978        0.023128       -1.358554
C                -1.690518       -1.458756        0.028993
C                -2.469263        0.673049       -1.028640
C                -3.722093       -1.357192       -1.310731
C                -2.744033       -2.080144       -0.605555
C                -1.411227       -0.107158       -0.382379
H                -4.608763       -1.890082       -1.642651
H                -2.939832       -3.128797       -0.393203
C                -1.105662       -2.114436        1.261119
H                -0.190050       -1.611840        1.565166
H                -0.859600       -3.158119        1.032990
C                -5.076494        0.685774       -1.493374
H                -5.755191       -0.091549       -1.856724
H                -5.120742        1.484527       -2.234532
C                -5.662090        1.227180       -0.126585
H                -6.752529        1.135377       -0.179066
H                -5.439964        2.295487       -0.028503
C                -2.079851       -2.131002        2.522781
H                -1.471397       -1.865109        3.393522
H                -2.438317       -3.153236        2.679619
C                -3.254047       -1.202471        2.370199
C                -5.078623        0.486987        1.049792
C                -4.508694       -1.680169        1.971012
C                -3.057625        0.183255        2.363780
C                -3.959659        1.015092        1.706365
C                -5.416852       -0.843610        1.320966
H                -4.732657       -2.741125        2.061080
H                -2.134504        0.598191        2.763159
H                -3.728473        2.073349        1.602808
H                -6.332326       -1.265374        0.911113
C                -2.225003        2.055491       -1.282905
C                -1.034528        2.594395       -0.833387
H                -0.815352        3.649183       -0.958051
C                -0.043646        1.765426       -0.314584
C                -3.140058        2.968379       -2.051352
H                -3.420600        2.532083       -3.013825
H                -2.636958        3.917383       -2.248662
H                -4.059002        3.194053       -1.503474
C                 1.274560        2.300019       -0.012880
O                 1.458071        3.612966        0.101593
C                 2.812444        3.771792        0.603427
H                 3.284614        4.574170        0.034500
H                 2.734878        4.054196        1.657241
C                 3.486584        2.386209        0.407105
N                -0.174050        0.442354       -0.149834
N                 2.291378        1.532278        0.148457
Ru                1.828419       -0.504767        0.087635
Cl                1.547220       -0.183280        2.458493
C                 1.952175       -1.525913       -1.985955
C                 3.267386       -2.212271        0.516679
C                 1.337514       -2.387427       -1.018234
C                 3.197464       -0.970324       -1.622157
C                 3.852115       -1.311807       -0.397396
C                 1.974909       -2.737069        0.188344
H                 0.336855       -2.759470       -1.203607
H                 3.672164       -0.256862       -2.287903
H                 4.805478       -0.855956       -0.153490
H                 1.467137       -3.372799        0.903675
C                 3.937437       -2.586957        1.799899
H                 4.294579       -3.621280        1.731283
H                 3.238845       -2.515242        2.637191
H                 4.792789       -1.942306        2.010539
C                 1.355458       -1.244177       -3.358568
H                 2.131005       -1.575061       -4.065498
C                 1.116419        0.250231       -3.610634
H                 0.823404        0.410103       -4.652573
H                 2.009495        0.853682       -3.423613
H                 0.311997        0.625155       -2.970952
C                 0.095134       -2.056214       -3.660671
H                -0.216240       -1.875104       -4.693322
H                -0.740003       -1.770825       -3.011980
H                 0.264157       -3.132903       -3.556878
C                 4.399149        2.389444       -0.822922
H                 3.855891        2.693432       -1.723274
H                 5.224201        3.091931       -0.667784
H                 4.837483        1.403393       -0.992879
```

C	4.239418	1.953484	1.660337
H	5.037690	2.672355	1.873135
H	4.698452	0.971756	1.522971
H	3.570261	1.891380	2.520524

$\mathbf{R}_P\mathbf{R}_M$-[3]$^+$: C4

80
Enegy: -2096.01418190

C	-3.779078	-0.079997	-1.224095
C	-1.718039	-1.489005	0.190430
C	-2.544267	0.599720	-0.920082
C	-3.763267	-1.457742	-1.136563
C	-2.769584	-2.142893	-0.414817
C	-1.466427	-0.147387	-0.268445
H	-4.641659	-2.016086	-1.448411
H	-2.948165	-3.187272	-0.169631
C	-1.123324	-2.108322	1.434915
H	-0.086030	-1.816124	1.586397
H	-1.158405	-3.196450	1.311284
C	-5.156074	0.550530	-1.385056
H	-5.811629	-0.248022	-1.744297
H	-5.206176	1.333143	-2.142450
C	-5.777106	1.107392	-0.036379
H	-6.853407	0.905909	-0.063808
H	-5.662390	2.196383	-0.003404
C	-1.891598	-1.750429	2.788594
H	-1.189844	-1.195287	3.417730
H	-2.116605	-2.690791	3.301937
C	-3.141835	-0.944196	2.572323
C	-5.113581	0.499311	1.172324
C	-4.362981	-1.545586	2.238786
C	-3.055006	0.447568	2.456122
C	-4.031271	1.159716	1.764683
C	-5.340184	-0.831742	1.545597
H	-4.506314	-2.609107	2.418453
H	-2.161465	0.959444	2.807024
H	-3.886848	2.222780	1.582588
H	-6.227853	-1.350083	1.188772
C	-2.319547	1.978409	-1.210457
C	-1.123105	2.540626	-0.804743
H	-0.918502	3.593709	-0.963319
C	-0.112165	1.735867	-0.285979
C	-3.264589	2.866200	-1.971599
H	-4.182281	3.070160	-1.413315
H	-3.545625	2.420143	-2.929583
H	-2.787459	3.826612	-2.177936
C	1.211826	2.284542	-0.030915
O	1.378583	3.601006	0.050910
C	2.803179	3.812668	0.228353
H	3.173922	4.300262	-0.678103
H	2.933644	4.475783	1.085152
C	3.412282	2.397064	0.450358
N	-0.231680	0.418784	-0.078434
N	2.240847	1.530044	0.122017
Ru	1.783240	-0.522382	0.034926
Cl	1.647601	-0.315427	2.424165
C	2.114493	-1.185981	-2.138159
C	2.883131	-2.502908	0.340132
C	1.241132	-2.080295	-1.456704
C	3.344767	-0.911566	-1.487394
C	3.734241	-1.544962	-0.272872
C	1.624951	-2.757381	-0.269713
H	0.237994	-2.241840	-1.836960
H	3.999939	-0.161830	-1.918131
H	4.674405	-1.283450	0.199993
H	0.929267	-3.435718	0.207270
C	3.280559	-3.189893	1.607015
H	3.939757	-2.563417	2.210264
H	3.814531	-4.114367	1.354288
H	2.409644	-3.448029	2.211784
C	1.809858	-0.568219	-3.487198
H	2.278980	0.425070	-3.492874
C	0.319347	-0.388468	-3.775962
H	0.190109	0.154610	-4.716680
H	-0.184709	0.177890	-2.987771

H	-0.192820	-1.349940	-3.890800
C	2.484310	-1.410062	-4.585715
H	2.060791	-2.419762	-4.620199
H	3.562918	-1.502150	-4.424739
H	2.328214	-0.946716	-5.564793
C	4.583445	2.161641	-0.500391
H	5.046410	1.188018	-0.322673
H	4.273097	2.232487	-1.547505
H	5.352528	2.920872	-0.325189
C	3.843526	2.193531	1.902926
H	4.672477	2.872638	2.129977
H	4.173694	1.167256	2.074106
H	3.021004	2.391885	2.593480

$\mathbf{R}_P\mathbf{S}_M$-[3]$^+$: C1

80
Enegy: -2095.97572900

C	-3.691949	-0.626152	1.423297
C	-1.776079	1.344108	0.644505
C	-2.526832	-1.036002	0.683402
C	-3.656487	0.630179	2.002684
C	-2.743908	1.617217	1.585085
C	-1.510510	-0.039819	0.385691
H	-4.481582	0.937554	2.639382
H	-2.935039	2.648073	1.875091
C	-1.273279	2.430034	-0.279487
H	-0.380513	2.072907	-0.794639
H	-0.998389	3.319548	0.298189
C	-5.052401	-1.309668	1.419674
H	-5.643231	-0.816040	2.196818
H	-5.020051	-2.363392	1.699594
C	-5.848939	-1.170235	0.054658
H	-6.910158	-1.060891	0.303021
H	-5.755619	-2.096924	-0.521919
C	-2.326698	2.915913	-1.377673
H	-1.800197	2.971217	-2.336865
H	-2.636337	3.935537	-1.127567
C	-3.538667	2.030032	-1.477650
C	-5.336858	-0.015638	-0.767610
C	-4.704807	2.323639	-0.758841
C	-3.450957	0.770032	-2.079855
C	-4.342143	-0.240030	-1.727798
C	-5.598883	1.312151	-0.409068
H	-4.855722	3.327169	-0.366297
H	-2.613289	0.539647	-2.735470
H	-4.185150	-1.245601	-2.112086
H	-6.430353	1.540345	0.254502
C	-2.328475	-2.352422	0.160757
C	-1.241061	-2.564687	-0.665824
H	-1.070443	-3.531860	-1.125556
C	-0.245889	-1.591247	-0.762483
C	-3.185526	-3.544183	0.483096
H	-4.188052	-3.469585	0.053205
H	-3.290060	-3.668174	1.564742
H	-2.725354	-4.452085	0.087458
C	1.048832	-1.922893	-1.335999
O	1.163764	-2.944156	-2.180061
C	2.544371	-2.925451	-2.620309
H	2.903255	-3.955291	-2.646608
H	2.558719	-2.497458	-3.628392
C	3.277030	-2.037335	-1.585171
N	-0.317814	-0.383157	-0.197326
N	2.121918	-1.287773	-1.004520
Ru	1.823857	0.083506	0.564915
Cl	1.306517	-1.875117	1.867215
C	2.434539	2.281126	0.052512
C	3.123906	0.635263	2.343634
C	3.544271	1.410007	0.027913
C	1.614064	2.219631	1.222315
C	1.942999	1.435791	2.347810
C	3.891188	0.602148	1.152312
H	4.151372	1.351069	-0.867575
H	0.696478	2.793150	1.250519
H	1.275167	1.405821	3.201416
H	4.753397	-0.053656	1.099096

C	3.519894	-0.162613	3.543512
H	4.110836	-1.038193	3.269216
H	2.646821	-0.501466	4.103042
H	4.128711	0.476343	4.196090
C	2.169872	3.277711	-1.056613
H	1.135974	3.620277	-0.943478
C	2.323036	2.697231	-2.464960
H	2.023643	3.442104	-3.208264
H	1.701054	1.807105	-2.601618
H	3.362010	2.429253	-2.686071
C	3.083362	4.500795	-0.853192
H	2.853639	5.268456	-1.598689
H	4.138549	4.228250	-0.965864
H	2.953319	4.944561	0.138854
C	3.924880	-2.888944	-0.489611
H	3.202494	-3.577462	-0.043668
H	4.314406	-2.260416	0.313736
H	4.754399	-3.465181	-0.912838
C	4.297206	-1.136863	-2.272661
H	4.978620	-1.748075	-2.873816
H	4.911080	-0.601679	-1.544493
H	3.811650	-0.415443	-2.936008

$\mathbf{R}_P\mathbf{S}_M$-$[\mathbf{3}]^+$: C2

80
Enegy: -2096.00436954

C	-3.691297	-1.013938	1.592148
C	-1.937630	1.125723	0.881683
C	-2.544231	-1.293528	0.768023
C	-3.693222	0.190078	2.272946
C	-2.861186	1.260280	1.893385
C	-1.606427	-0.215199	0.496475
H	-4.498439	0.396328	2.972463
H	-3.097532	2.250844	2.275703
C	-1.565947	2.314668	0.019026
H	-0.810504	1.996370	-0.701024
H	-1.134542	3.121242	0.622748
C	-5.012757	-1.769619	1.589590
H	-5.595058	-1.368629	2.424410
H	-4.916022	-2.838510	1.784175
C	-5.869814	-1.569289	0.272391
H	-6.926105	-1.600652	0.560864
H	-5.703942	-2.412413	-0.406908
C	-2.785384	2.948460	-0.777775
H	-2.395109	3.304706	-1.738355
H	-3.140640	3.831143	-0.236500
C	-3.929197	1.984835	-0.958037
C	-5.506957	-0.285157	-0.428252
C	-5.079069	2.084127	-0.165095
C	-3.764050	0.817227	-1.711190
C	-4.543626	-0.304644	-1.445167
C	-5.866478	0.962177	0.093965
H	-5.292851	3.015135	0.355784
H	-2.941412	0.739396	-2.419464
H	-4.316654	-1.241309	-1.949687
H	-6.679762	1.035742	0.812790
C	-2.290880	-2.558432	0.152855
C	-1.228503	-2.650795	-0.726619
H	-1.016490	-3.576575	-1.249460
C	-0.307418	-1.607584	-0.811979
C	-3.058115	-3.819934	0.433923
H	-4.079850	-3.785460	0.046396
H	-3.110891	-4.013587	1.508930
H	-2.558669	-4.671212	-0.033148
C	0.969901	-1.809364	-1.477912
O	1.113764	-2.815752	-2.333492
C	2.463482	-2.707009	-2.845812
H	2.908557	-3.703162	-2.831592
H	2.391611	-2.345556	-3.876461
C	3.173822	-1.696757	-1.906503
N	-0.430287	-0.441259	-0.171327
N	1.999726	-1.074902	-1.220683
Ru	1.685962	0.184360	0.443112
Cl	1.518353	-1.896953	1.651929
C	2.835569	2.111887	-0.210274

C	2.168436	1.150872	2.455495
C	3.667238	1.168059	0.477508
C	1.636175	2.469021	0.429610
C	1.304774	1.995524	1.738383
C	3.347267	0.698010	1.768843
H	4.564774	0.796652	-0.005813
H	0.945367	3.125933	-0.080822
H	0.353511	2.269197	2.181023
H	3.976600	-0.050542	2.238253
C	1.859733	0.682164	3.840879
H	2.031015	-0.393202	3.933430
H	0.823133	0.892962	4.111151
H	2.514218	1.201192	4.551252
C	3.271496	2.731356	-1.520046
H	3.956262	2.024011	-1.999610
C	4.071108	4.011924	-1.214419
H	4.463020	4.438714	-2.142711
H	4.918598	3.815010	-0.550465
H	3.436075	4.766490	-0.737864
C	2.126006	3.011917	-2.494661
H	2.531127	3.346777	-3.453993
H	1.467673	3.809981	-2.134799
H	1.520061	2.118408	-2.673963
C	4.046700	-2.414891	-0.874736
H	3.469815	-3.152938	-0.312292
H	4.464647	-1.707661	-0.154648
H	4.876527	-2.917568	-1.382502
C	3.983864	-0.699572	-2.726953
H	4.687940	-1.240981	-3.367594
H	4.575470	-0.041873	-2.087590
H	3.338863	-0.090890	-3.366819

$\mathbf{R}_P\mathbf{S}_M$-$[\mathbf{3}]^+$: C3

80
Enegy: -2096.00430484

C	-3.405430	-0.863719	1.662451
C	-1.547880	1.166053	0.895986
C	-2.301740	-1.212358	0.806364
C	-3.315222	0.338830	2.339928
C	-2.430875	1.355894	1.934655
C	-1.310046	-0.191762	0.501168
H	-4.085947	0.593926	3.061860
H	-2.593497	2.358576	2.323538
C	-1.131297	2.332605	0.023998
H	-0.424956	1.968831	-0.723916
H	-0.627460	3.105883	0.614977
C	-4.770235	-1.537134	1.697493
H	-5.304145	-1.100836	2.546859
H	-4.734374	-2.609944	1.891146
C	-5.648292	-1.284872	0.403400
H	-6.696832	-1.257087	0.719273
H	-5.547861	-2.134273	-0.280820
C	-2.334817	3.046530	-0.726961
H	-1.954813	3.389109	-1.696675
H	-2.619482	3.943095	-0.167096
C	-3.538865	2.153549	-0.877065
C	-5.231089	-0.021893	-0.305375
C	-4.658031	2.317634	-0.051695
C	-3.463705	0.980499	-1.636047
C	-4.299555	-0.094686	-1.349224
C	-5.502385	1.242957	0.227971
H	-4.801896	3.257859	0.476580
H	-2.667228	0.856539	-2.367278
H	-4.141723	-1.041654	-1.860850
H	-6.289315	1.361977	0.969690
C	-2.143405	-2.491925	0.190019
C	-1.118041	-2.648634	-0.723106
H	-0.977561	-3.586688	-1.248146
C	-0.142651	-1.659943	-0.846795
C	-2.973398	-3.705561	0.502139
H	-4.001423	-3.615695	0.140765
H	-3.008796	-3.888683	1.579642
H	-2.535722	-4.587049	0.029136
C	1.091377	-1.936925	-1.565033
O	1.139476	-2.953123	-2.419451

C	2.472257	-2.934696	-2.983879
H	2.861739	-3.953716	-2.955307
H	2.380806	-2.600472	-4.021877
C	3.275465	-1.939485	-2.102794
N	-0.173820	-0.486575	-0.207906
N	2.171062	-1.260607	-1.359512
Ru	2.012064	0.017424	0.308238
Cl	1.771828	-2.044768	1.538513
C	2.702129	0.943361	2.289611
C	3.202958	1.881197	-0.421489
C	1.826908	1.835227	1.647463
C	3.793446	0.434088	1.503240
C	4.038048	0.892767	0.191220
C	2.078538	2.293361	0.315123
H	0.926280	2.157936	2.155626
H	4.418900	-0.348867	1.919116
H	4.873306	0.477590	-0.362076
H	1.390609	2.991518	-0.143751
C	3.513343	2.480215	-1.759505
H	2.607225	2.824460	-2.263749
H	4.031832	1.780970	-2.416043
H	4.168028	3.349109	-1.620317
C	2.535460	0.478122	3.716642
H	2.800168	-0.586097	3.723758
C	1.113159	0.608108	4.256723
H	1.059476	0.156212	5.251216
H	0.394891	0.089896	3.615370
H	0.807303	1.655378	4.364095
C	3.545810	1.236899	4.597800
H	3.496301	0.858607	5.623148
H	3.322792	2.309197	4.623151
H	4.575251	1.112696	4.246516
C	4.180747	-2.677504	-1.114201
H	3.608232	-3.377187	-0.500456
H	4.676727	-1.977485	-0.437945
H	4.952485	-3.227683	-1.662639
C	4.069973	-0.984366	-2.987381
H	4.721527	-1.559992	-3.653202
H	4.715149	-0.331376	-2.396744
H	3.408137	-0.370505	-3.605032